ENVIRONMENTAL SECURITY TECHNOLOGY CERTIFICATION PROGRAM

FINAL TECHNICAL REPORT, VOLUME I

FOR

APPLICATION OF FLOW AND TRANSPORT OPTIMIZATION CODES TO GROUNDWATER PUMP AND TREAT SYSTEMS

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TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF APPENDICES

ACRONYMS

1,1,1-TCA	1,1,1-Trichloroethane
1,1-DCE	1,1-Dichloroethylene
ACLs	alternate concentration limits
AFCEE	Air Force Center for Environmental Excellence
AEHS	The Association for Environmental Health and Sciences
ANN	artificial neural network
ASCE	American Society of Civil Engineers
BMC	Bomb and Mine Complex
BRAC	Base Realignment and Closure
COC	contaminant of concern
CPU	central processing unit
DCE	1,2-Dichloroethane
DoD	Department of Defense
DRMO	Defense Reutilization ad Marketing Office
EDA	Explosives Disposal Area
ESTCP	Environmental Security Technology Certification Program
FS	feasibility study
FY	fiscal year
GA	genetic algorithm
GAC	granular activated carbon
Ghz	gigahertz
gpm	gallon per minute
GUI	graphical user interface
HEIP	Hastings East Industrial Park
HGCS	Hastings Groundwater Contamination Site
IWL	Industrial Wastewater Lagoon
ITR	Independent Technical Review
MCLs	maximum concentration limits
NARPM	National Association of Remedial Project Managers
NFESC	Naval Facilities Engineering Service Center
NPL	National Priorities List
NPV	net present value
O&M	operating and maintenance
OU	operable unit
P&T	pump-and-treat
PC	personal computer
PCE	Tetrachloroethylene
POE	Point of Exposure
POC	Point of Compliance
ppb	part per billion
RCRA	Resource Conservation and Recovery Act
RDX	Royal Demolition Explosive
RI	remedial investigation
RPO	Remedial Process Optimization

RSE	Remediation System Evaluation
SA	simulated annealing
SERDP	Strategic Environmental Research & Development Program
SVE	soil vapor extraction
TCE	Trichloroethylene
TIO	Technology Innovation Office
TNT	2,4,6-Trinitrotoluene
TS	tabu search
UA	University of Alabama
UMass	University of Massachusetts
USACE	United States Army Corps of Engineers
HTRW-CX	Hazardous, Toxic, and Radioactive Waste Center of Expertise
USDA	United States Department of Agriculture
US EPA	United States Environmental Protection Agency
USU	Utah State University
VOCs	volatile organic compounds
WWII	World War II
YD	Yard Dump

1. Introduction

1.1 Background Information

A 1998 Department of Defense (DoD) Inspector General report (*DoD IG*, 1998) indicates that the cumulative operating and maintenance (O&M) costs for 75 pump and treat systems operating at DoD chlorinated solvent groundwater sites (a subset of over 200 DoD pump and treat sites) was $40 million in fiscal year (FY) 1996. The report also projected that these costs would reach $1 billion by the year 2020. Recent studies completed by the EPA (*EPA*, 2002) and the Navy (*NAVFAC*, 2003) indicate that the majority of pump and treat systems are not operating as designed, have unachievable or undefined goals, and have not been optimized since installation. Even under ideal circumstances, (i.e., when the initial pump and treat system has been appropriately designed with clearly-defined objectives), changes in contaminant distributions and aquifer stresses, coupled with evolving regulatory climates, result in the need for system optimization.

Although it is recognized that many of these pump and treat systems are ineffective for cleanup, regulations require that they continue to operate until a more effective solution is developed. In the interim, the potential for tremendous cost savings exists with the application of simple screening tools and optimization-simulation modeling (*US EPA*, 1999a,b). The optimization-simulation models link mathematical optimization techniques with simulations of groundwater flow and/or solute transport, to determine the best combination of well locations and pumping rates.

1.2 Official DoD Requirement Statement(s)

1.2.1. List of the Requirements

Table 1-1 lists the DoD needs requirements related to optimization of pump and treat systems.

Table 1-1. DoD Needs/Requirements

Service	Requirement Number	Requirement Title	Priority H,M,L
Army	A(1.5.o)	Development of Predictability Model for In-Situ Groundwater Treatment (Containment-Movement)	L
Air Force	2008	Methods and Remedial Techniques are Needed to More Effectively Treat Groundwater Contaminated with Chlorinated Solvents	M

Navy	1.I.1.e	Improved remediation of groundwater contaminated with non-chlorinated hydrocarbons	M
Navy	1.I.1.g	Improved remediation of groundwater contaminated with chlorinated hydrocarbons and other organics	H
Navy	1.II.1.a	Improved fate, effects and transport model for groundwater	M

1.2.2. How Requirement(s) Were Addressed

The optimization of groundwater pump and treat systems using mathematical algorithms contributes potentially to long-term operating cost reduction and improved performance of these systems with respect to compliance objectives. Algorithmic approaches can be applied to the redesign of pump and treat systems that address any contaminant type in the groundwater, so long as the groundwater model effectively represents the historical and current plume capture boundaries, as well as the flow and transport properties of the aquifer and the contaminants. For this project, two of the three sites specifically address chlorinated hydrocarbons, and two of three sites address non-chlorinated hydrocarbons. Finally, this approach also can reveal uncertainties or data gaps associated with the existing groundwater flow and transport model for a site that are critical for evaluating the effectiveness of the P&T system, which in turn indicates priorities for additional data collection.

1.3 Objectives of the Demonstration

The primary objective of this project is to demonstrate the cost benefit of applying transport optimization codes to existing pump and treat systems relative to the traditional trial-&-error approach. The transport optimization codes couple sophisticated nonlinear optimization techniques with simulations of groundwater flow and solute transport. A secondary objective is to provide each installation where the demonstration is performed with alternate pumping strategies that are feasible and cost-effective to implement. While the installations are encouraged to implement optimization suggestions resulting from the demonstration, they are not required to do so, and comparing current performance data to future performance field data from the actual "optimized" system is not a primary objective of this demonstration.

A previous project, which was sponsored by the US EPA (*US EPA*, 1999a,b) demonstrated potential avoidance of millions of dollars in O&M costs over the projected lifetime of the pump and treat system at two of three sites through the application of hydraulic optimization. Hydraulic optimization couples simpler optimization techniques (linear and mixed-integer programming) with simulations of groundwater flow (but not transport). The transport optimization techniques that are the focus of this ESTCP project are potentially more powerful than the hydraulic optimization techniques, because they

rigorously incorporate predictions of contaminant concentrations, contaminant mass, and/or cleanup duration. However, transport optimization codes are also more complex and difficult to apply than hydraulic optimization codes.

This demonstration project was divided into two phases:

- Phase 1: Pre-optimization site screening
- Phase 2: Demonstration of transport optimization codes

For Phase 1, a spreadsheet-based pre-optimization screening methodology was developed and applied at eleven existing pump and treat systems at DoD (Appendix G). The objective of Phase 1 was to provide end-users with a framework and a simple tool for quickly and inexpensively prioritizing which sites are most likely to benefit from the application of transport optimization codes. The pre-optimization screening methodology developed in Phase 1 can be used for both existing and planned systems. For this project, additional criteria for site selection included the existence of a flow and transport model and a willingness to consider implementing changes suggested by the optimization analysis.

For Phase 2, transport optimization was performed for three sites (Figure 1-1):

- Umatilla Chemical Depot, Hermiston, Oregon (“Umatilla”)
- Tooele Army Depot, Tooele, Utah (“Tooele”)
- Former Blaine Naval Ammunition Depot, Hastings, Nebraska (“Blaine”)

Details of procedures and results for Phase 2 are presented in this report. Both Umatilla and Tooele sites have existing P&T systems in operation, and the Blaine site is a planned P&T system. The use of the optimization algorithms in Phase 2 is applicable to both new and existing P&T systems.

The demonstration utilized existing groundwater flow and transport models for each site. A pre-requisite of selecting a site for inclusion in the project was the existence of a numerical transport model considered to be “up-to-date and acceptable for design purposes”, based on previous conceptual model development and model calibration activities (which are specifically not within the scope of this project because this project is intended to evaluate the optimization algorithms and not the quality of the underlying models). Due to project scheduling and resources, and the evolving nature of the groundwater models, it was necessary to proceed with a model that was current at a specific point in time, even if future recalibration was anticipated.

It is noted that a numerical groundwater model will never exactly predict groundwater flow and contaminant transport, and that any results obtained based on groundwater model predictions must be evaluated in that context. However, those issues pertain equally to any design based on flow and transport modeling, whether obtained using transport optimization algorithms or trial-&-error techniques. This project did not evaluate the impact of the uncertainty associated with simulation model parameters on

the optimization solutions. However, this issue could be evaluated in future projects either by examining the impact to optimal solutions from varying model parameter values or by using stochastic optimization methods to identify optimal solutions that are robust despite the uncertainty. Optimal solutions are often "at the edge" of what is feasible and therefore are not always robust. This project was not designed to evaluate the robustness of the optimal solutions. One way to increase the robustness of the solutions would be to apply a "safety factor" to the optimization problem (i.e., impose more restrictive constraints than are actually required), which in general will lead to more conservative designs.

1.4 Regulatory Issues

At this time, there are no technology-specific regulatory issues that need to be directly addressed beyond those that constrain the design and operation of the pump and treat systems being examined, e.g., such as hydraulic capture boundaries and overall revision of pump and treat system objectives. Those regulatory issues were represented by the installation and considered during the strategic development of the mathematical formulations that were solved using the transport optimization algorithms. The ESTCP project team encouraged regulatory participation in the process and for each demonstration site offered to help site personnel communicate with their regulatory partners regarding the optimization technology. However, installation personnel were ultimately responsible for keeping regulators involved in the project to the extent desirable and necessary. Some of the facility-specific regulatory issues encountered during the project are described in later sections of the document where the demonstration sites are discussed individually. The ESTCP project team may continue to offer technical assistance for obtaining regulatory approval to implement the results of this technology demonstration as requested by the facility.

1.5 Previous Testing of the Technology

Since the 1980's, many researchers have sought to couple groundwater simulation models with mathematical optimization techniques to address groundwater management issues. Several universities have developed transport optimization codes, and some have been tested at actual field sites. Three examples of recent applications of transport optimization are:

- Utah State University: Wurtsmith Air Force Base
- University of Alabama: Massachusetts Military Reservation (CS-10)
- Utah State University: Massachusetts Military Reservation (CS-10)

Each is described below. Peralta (2001) describes other recent real-world design and implementation projects using earlier versions of the Utah State University model.

Wurtsmith Air Force Base, MI: Optimizing Contaminant Mass Removal Using Artificial Neural Network – Utah State University.

In this case (*Aly, A.H. and R.C. Peralta,* 1997), transport optimization was used to develop an optimal strategy for remediating TCE and DCE groundwater plumes. Management goals and restrictions were identified and prioritized as follows:

- Capture the TCE and DCE dissolved phase groundwater plumes
- Reduce TCE and DCE concentrations to less than 94 ppb and less than 230 ppb, respectively, within 6 years
- Total extraction of groundwater cannot exceed 400 gpm
- No treated water may be injected into the groundwater
- Treatment facility effluent cannot exceed 5 ppb of TCE

An artificial neural network was used to simulate contaminant concentrations in the optimization model. The model considered a total of 24 potential extraction well locations. Six alternative optimal pumping strategies were ultimately evaluated for the final design. After discussions with stakeholders, a final strategy was chosen based on its minimization of total pumping rates, minimization of total time to meet objectives, and overall benefit to the stakeholders.

Chemical Spill-10 (CS-10) site located at the Massachusetts Military Reservation – University of Alabama and Utah State University

Two of the three recent study applications of transport optimization were applied for the CS-10 plume at Massachusetts Military Reservation. A pump and treat system is operating to remediate and contain a TCE plume approximately 17,000 feet long, 6,000 feet wide, and up to 140 feet thick. Between Fall 1999 and Spring 2000, transport optimization codes were utilized to maximize TCE mass removal over a 30-year time horizon, subject to the following constraints: (1) the TCE concentration must be lower than or equal to 5 ppb beyond the base boundary, (2) all extracted water must be reinjected into infiltration trenches, (3) individual wells are subject to pumping capacities, and (4) the total pumping rate should be restricted for cost considerations. The decision variables were the extraction rates and well locations for four perimeter wells that were being considered, and the extraction rates for five in-plume wells that were already constructed.

Results for the two optimization studies are summarized below:

- *University of Alabama*. In this case (*AFCEE,* 1999; *Zheng and Wang,* 2002), the optimal strategy, as determined by the simulation-optimization analyses, suggests using only one perimeter well (rather than four wells) and a maximum pumping rate of 2700 gallons per minute (gpm). The results of the analysis demonstrate that it is possible to remove more TCE mass (approximately 3.5%) under the same amount of pumping assumed in the trial and error design, and that it can also lead to substantial cost savings by reducing the number of wells needed and adapting dynamic pumping. Preliminary cost estimates indicated that this strategy would yield life cycle cost savings of $2.4 million. Some elements of the design were implemented.

- *Utah State University*. In this case (*Peralta et al*, 1999a, b), the simulation-optimization modeling enhanced mass removal rates and aided in well placement, with an additional constraint of preventing the plume from contaminating clean aquifer between the western and central lobes. Specifically, the modeling identified a configuration that would extract approximately 6% more mass over 30 years, while reducing the extraction rate by 50 gpm and could cost $0.54M less in installation cost alone. With slight tweaking, this design was constructed and is functioning as expected.

1.6 Project Team, Roles and Overall Project Coordination

This project was coordinated by the following Management Team:

- US Navy (Karla Harre, Laura Yeh, Nick Ta, Paul Lefebvre, Doug Zillmer)
- US EPA Technology Innovation Office (Kathy Yager)
- US Army Corp of Engineers (USACE) HTRW-CX (Dave Becker)
- GeoTrans, Inc. (Rob Greenwald, Yan Zhang)
- Barbara S. Minsker Consulting (Barbara Minsker, PhD)

The Navy served as the primary interface with the ESTCP, provided technical oversight, and was also responsible for contracting with the following organizations that performed the actual transport optimization simulations:

- University of Alabama (Chunmiao Zheng, PhD), herein referred to as the "UA team"
- Utah State University (Richard Peralta, PhD), herein referred to as the "USU team"

The transport optimization contractors were selected based on a bid proposal process. Selection was performed by a committee consisting of the US Navy, the USEPA, and the USACE. In addition to performing the transport optimization at each site, Dr. Zheng and Dr. Peralta provided input for evaluating the existing models and developing the optimization formulations for each site.

The USEPA provided technical oversight and offered to interface with regulators when requested, and was also responsible for contracting with GeoTrans and Dr. Minsker in the early stages of the project. The USACE provided technical oversight and was responsible for identifying all three sites ultimately selected for the demonstration. Therefore, USACE also served as the primary interface between the Management Team and the individual installations for all aspects of the project (site visits, evaluating models, developing formulations, and presenting results). GeoTrans was the technical lead for developing and implementing the site screening methodology, evaluating the existing groundwater models for each site, and developing the optimization formulations (in conjunction with the installations). GeoTrans also performed the trial and error modeling for each site, serving as the scientific control for the transport optimization. Dr. Minsker provided technical oversight and was primarily responsible for interpreting the results with respect to the project objectives. The Navy has provided contractual and administrative support as the DoD lead on this project, and is responsible for the accuracy and quality of the project results and conclusions as reflected in the final project documentation submitted to the ESTCP office.

1.7 Document Organization

This document is organized according to the ESTCP-suggested format guidelines as follows:

- Section 1: Introduction
- Section 2: Technology Description
- Section 3: Site/Facility Description
- Section 4: Demonstration Approach
- Section 5: Performance Assessment
- Section 6: Cost Assessment
- Section 7: Regulatory Issues
- Section 8: Technology Implementation
- Section 9: Lessons Learned
- Section 10: References

Section 3 includes a screening tool methodology that was developed to select the 3 sites that were investigated in this mathematical optimization project. In each section where site data or site specific results are discussed (such as Sections 3 through 5), data is organized by site within each subtopic or subsection. Detailed results and supplemental information have been provided in Appendices A through G.

2. Technology Description

2.1 General Description

This project demonstrates the application of transport optimization codes, which couple nonlinear optimization algorithms with existing groundwater flow and transport models, to determine an optimal set of well locations and pumping rates for a specific "formulation". A formulation includes:

- An objective function to be minimized or maximized
- A set of constraints that must all be satisfied

During transport optimization, the formulation can be solved using mathematical algorithms to find the best or near-best combination of pumping rates and well locations (called the "optimal solution" or "near optimal solution"). The objective function might be formulated to minimize costs, maximize mass removal, minimize mass remaining in the aquifer, or minimize cleanup time. Constraints might include limits on pumping rates at specific wells, limits on total amount of water extracted for treatment, restrictions on well locations, limits on water levels or drawdowns, limits on contaminant concentrations, limits on capital investment, and many other physical and/or economic restrictions.

Most pump and treat systems have been designed through the use of numerical flow and/or solute transport simulation models, such as MODFLOW and MT3D. Traditionally, the groundwater simulation model is run repeatedly to simulate different pumping scenarios (referred to as "trial and error"). Each pumping scenario is entered manually, building on the results of the previous simulations and determined largely on the experience and insight of the modeler. Using this trial and error approach, a limited number of simulations are performed (typically 10 to 50) and a preferred pumping strategy is then selected. A limitation of this approach is that only a small number of possibilities can be feasibly investigated, and the objectives and constraints are often not rigorously stated (in mathematical terms). Another limitation is that the nonlinear nature of the transport model (i.e., concentrations do not change proportionally with pumping rates) complicates selecting wells locations and pumping rates based on earlier choices.

Transport models incorporate contaminant advection, dispersion, adsorption, and reaction, allowing for prediction of concentration, mass, and cleanup times. Transport optimization codes (the focus of this demonstration project) couple these transport models with nonlinear mathematical optimization, to allow a systematic evaluation of potential pumping strategies (i.e. using mathematical algorithms instead of manual iteration). Nonlinear optimization algorithms are required because concentration changes and/or cleanup time changes are not linearly related to pumping rate. This approach is therefore a coupled simulation-optimization approach.

The nonlinear optimization problem that results from the transport optimization formulations can be conceptualized as a mountain range with a series of peaks and valleys. The optimal solution is either the highest peak or the lowest valley, depending on the nature of the objective function (maximize or minimize). There are many algorithms for solving these nonlinear problems. Most traditional approaches use derivatives of the objective function and constraints to go “uphill” from the starting point of the search until the peak is found. These approaches find only the highest peak or lowest valley nearest the starting point of the search. They are also difficult to implement with complex transport models, which may not be differentiable. This project demonstrates global optimization methods, which are less susceptible to these limitations.

The coupled simulation-optimization approach is appealing because it can account for many complexities of the groundwater flow and contaminant transport (using the transport model), and it can presumably identify improved pumping strategies for a given objective function and constraint set by more efficiently searching the range of potential combinations of well rates and locations (using one or more nonlinear optimization algorithms). The performance objective of this project is to demonstrate the cost benefit of applying transport optimization codes, by addressing the following questions:

- Do the results obtained from these optimization software packages (e.g. recommended optimal pump and treat scenarios) differ substantially from the optimal solutions determined by traditional “trial-and-error” optimization methods?

- Do the results obtained from these optimization software packages warrant the additional effort and costs when compared to traditional “trial-and-error” optimization methods?

The objective function associated with each formulation is designed to be a metric for comparing one solution to another within the optimization approach, and therefore is ideally suited for measuring performance when the constraints are satisfied. More details regarding the performance objective and design of the study are presented in Section 4.1 and 4.2.

2.2 Global Optimization Methods

A new class of optimization methods, referred to as “heuristic global optimization methods”, has emerged in recent years. These methods include simulated annealing, artificial neural networks, genetic algorithms, outer approximation, and tabu search. These global methods are designed to search the potential solution space for the highest peak or lowest valley. These global methods often require intensive computational effort, but have become more practical for application on personal computers as computer speeds have increased. They can also handle any form of objective function and constraints and any type of simulation model, along with relatively straightforward

linking of simulation models with the optimization algorithm. The transport optimization codes demonstrated in this project use a variety of global optimization methods.

These optimization approaches are briefly summarized below, along with references for further information.

Genetic Algorithms

Genetic algorithms are search techniques developed by *Holland* (1975) that simulate the mechanisms of natural selection in searching through the decision space for optimal solutions (*Goldberg*, 1989). Simple genetic algorithms consist of three basic operations: (1) selection, (2) crossover (mating), and (3) mutation (see *Goldberg*, 1989, for reference). In using genetic algorithms, a population of candidate solutions, or "strings", are formed, which are typically binary representations of different decisions. For this project, each string (called a chromosome) could be a binary representation of one set of pumping rates and well locations. These strings are then evaluated on their performance (fitness) with respect to the objective function and constraints, which in this project requires running the flow and transport simulation models for the candidate pumping rates and well locations. Using this fitness value, strings are selected to enter the mating population using one of a number of selection approaches that favor strings with higher fitness ("survival of the fittest"). The crossover or mating operation involves randomly assigning a mating partner from within the mating population to each string. Mating between the two strings takes place with a specified probability. If mating does not occur, the parent strings survive into the next generation. When mating does occur, one or more random crossover locations are selected on the strings and genetic information is exchanged between the two parent strings at the crossover location(s) to form two children. The parents are then replaced in the population by the children to keep a stable population size. Finally, mutation occurs when the bits of a string, called genes, are randomly changed with a specified probability. By repeating these three basic operations for a number of generations (requiring many iterations of the simulation model), the performance of the population continues to improve.

The general theory behind this process is that strings with high fitness values contain information chunks ("building blocks") that are important to optimizing the objective function. By exchanging important building blocks between two strings that perform well, the genetic algorithm attempts to produce children strings which contain the important building blocks from both parents and, therefore, perform even better than the parent strings. In this way genetic algorithms use Darwin's "survival of the fittest" theory to search through the decision space for the best solutions. It is through this process of assembling strings with important building blocks that an optimal solution is found.

Simulated Annealing

Simulated annealing mimics the thermodynamic process in which a solid in a heat bath is initially heated to a liquid by increasing the temperature such that all the particles are

distributed randomly in a liquid phase. This is followed by slow cooling such that all the particles arrange themselves in the state of minimum energy where crystallization occurs. If the cooling is rapid, the system does not reach a highly ordered state, but ends up in a higher-energy state. *Metropolis et al.* (1953) introduced a simple algorithm to incorporate these ideas into optimization. The temperature is held fixed for a certain number of configuration changes and then lowered. At first, a higher value of temperature allows the algorithm to jump out of local minima and continue searching for a better configuration. Later, a lower temperature tends to confine the search to a local area, allowing the algorithm to converge.

Simulated annealing is a convenient way to find a global extremum of a function that has many local extrema and may not be smooth. The objective function to be minimized represents the energy in thermodynamic processes, while the optimal solution corresponds to the crystal configuration. The basic concept of simulated annealing lies in allowing the procedure to move occasionally “uphill”(i.e., a solution which does not lead to a better objective function), increasing the likelihood a global minimum will be found.

Tabu Search

Tabu search is another heuristic global optimization method that is based on an analogy to human memory. The current form of tabu search is based on the work of *Glover* (1986 and 1989) and involves sequential search with a short-term memory (tabu list) of solutions that were recently considered. Starting with a feasible solution, a set of nearby solutions (in terms of similar well locations and pumping rates) is first checked with the tabu list and rejected if it has recently been considered. The new solutions are then evaluated with respect to the objective function and constraints. The best solution then enters the tabu list and becomes the current solution. This process continues until all nearby solutions are labeled as tabu, at which point the algorithm starts at a new point. A long-term tabu memory is used to select new points in a way that encourages exploration of new solution regions. The long-term tabu memory records the frequency with which each solution variable’s value (e.g., each well location) has been used in the search. In generating new solutions, values that have been used least frequently have the highest probability of being selected. This process ensures that new solution regions are explored and creates the global search capabilities of the algorithm.

Artificial Neural Networks

The last approach used in this project is artificial neural networks, which were not used as an optimization algorithm but as a surrogate to the computationally-intensive simulation models during the optimization process. Many different types of artificial neural networks exist, but the most commonly used are called multilayer feedforward neural networks (*Rumelhart*, 1987). These types of neural networks essentially create highly generalized nonlinear regression models, in which a set of weights are fit (“trained”) to a set of input and output (“training”) data. In this project, the inputs could be pumping rates and the outputs contaminant levels at points of compliance, with the training data coming from runs of the flow and transport simulation models. Artificial neural networks have

been shown to be universal function approximators, if the appropriate structure is used. Multilayer neural networks consist of an input layer, an output layer, and one or more hidden layers. The input layer is the first layer, which receives the input data and scales them to ensure the values remain within a reasonable range (often between 0 and 1). The output layer is the last layer, which produces the output predictions. The hidden layers contain nodes (neurons) that transform the data using a number of predefined mathematical functions, such as a Gaussian function or sigmoid function. The neurons are linked in a network, with each connection in the network having a weight between 0 and 1. The weights are adjusted during training, but the structure of the neural network (numbers of layers, numbers of nodes in each layer, connections between the layers, and functions employed at each neuron) must be determined a priori using expertise and some experimentation. See *Principe et al.* (1999) for more details.

The artificial neural network is used as a response function to replace the simulation model within the optimization algorithms. Using the artificial neural network allows more potential solutions to be considered by the optimization algorithm because it estimates the results of the simulation faster than the full numerical simulation could be performed. However, the estimated results from the artificial neural network may not completely mimic the simulation model, such that solutions that appear feasible may actually not be feasible. Hence, solutions produced using an artificial neural network should always be tested with the full transport model after optimization.

2.3 Strengths, Advantages, and Weaknesses

A properly defined optimization problem can be solved through manual trial and error adjustment or using a formal optimization technique. While the trial and error method is simple and widely used, it is usually limited in practice to a small number of simulations (typically 10-50) because it is labor intensive. The transport optimization codes more efficiently evaluate the potential solution space, such that thousands of simulations are typically performed automatically, and each successive round of new simulations is designed to be "more promising" than the previous round.

Key advantages of transport optimization codes include the following:

- many more combinations of extraction and injection well rates can be evaluated using search algorithms that are far more efficient than trial-and-error or random search

- the process of mathematically specifying an objective function and a set of constraints is required for transport optimization, and this process (frequently overlooked during trial and error modeling) forces competing goals and strategies to be considered and compared

- because it is more automated than trial and error, transport optimization is less prone to bias in selecting well rates and well locations, and is therefore more likely to discover unexpected solutions

Limitations of transport optimization codes include:

- the site must develop a transport model that is considered a reasonable predictor for design purposes

- the complexity of applying the nonlinear transport algorithms requires specialized expertise for most real-world problems

- the codes are very computer intensive, potentially requiring simplification of the simulation model and/or dedicated use of one or more computers

A limitation that pertains to both trial and error and the use of transport optimization algorithms is that the optimal results are based on model predictions, which are subject to uncertainty. A number of approaches exist for considering uncertainty in the optimization process, but these were not evaluated in this project.

2.4 Factors Influencing Cost and Performance

One factor expected to affect the cost and performance of transport optimization is the time required to complete each model simulation (since thousands of simulations are generally performed for each optimization formulation). The simulation time is influenced by the model grid size (rows, columns, layers), heterogeneity within the model, the number of contaminants that must be simulated, the timeframe that must be simulated, and the time stepping that must be utilized to maintain accuracy within the numerical model. For this demonstration project, limits were placed on the simulation time (no more than two hours per transport simulation) and the number of contaminants rigorously simulated with the transport model (no more than two).

The flexibility to use different nonlinear optimization algorithms within a specific integrated code may also impact cost and performance. Different algorithms may be more efficient for different types of problems, so the ability to select from multiple algorithmic approaches is advantageous. Also, some optimization codes contain algorithms for fitting surrogate functions to the simulation model, such as artificial neural networks. The surrogate functions, which can be evaluated much more quickly than the original simulation model, are then used in place of the simulation model for optimization. For time-consuming simulation models, these approaches can reduce computational times and allow more strategies to be evaluated, but they can also introduce additional error. They also require expertise to implement appropriately.

3. Site/Facility Description

3.1 Background

In this project, a screening method was developed for site selection (Appendix G). The screening analysis is a two-stage procedure:

- first, answers to three simple questions suggest whether or not the site is likely to benefit from hydraulic and/or transport optimization

- then, if the user is interested in quantifying the potential cost savings from hydraulic and/or transport optimization, the second stage allows quick and inexpensive cost comparison of competing alternatives

The first stage is intended to quickly remove sites from consideration if they are not likely to benefit from either hydraulic or transport optimization. The three simple screening questions are:

- Are O&M costs > $100K/year?
- Is the system flowrate > 50gpm?
- Is the estimated cleanup time > 5 years?

If the answers to all three questions are "Yes", a potential benefit from hydraulic and/or transport optimization is suggested, and the second stage (i.e., quantitative potential cost saving evaluation) is recommended.

In the second stage, the potential cost savings are calculated based on site-specific values estimated by the user for hydraulic or transport optimization code application, whichever is most applicable, considering any potential model development and modification. However, for the purpose of this demonstration project, the existence of a sufficiently representative groundwater simulation model was required. Then classification of sites is primarily based on potential cost savings calculated for specific scenarios. Information provided by the user includes:

- basic information regarding the current pump-and-treat system (e.g., objectives, costs, pumping rate, number of wells, status of modeling efforts, etc.)

- estimated cost changes for specific scenarios associated with modified pumping rates and/or modified number of wells (including the costs of potential model development or modification)

Potential cost savings are estimated based on the total costs (NPV) for each alternative and the total cost of a baseline system (typically the existing or currently planned system) under three scenarios. The first two alternative scenarios assume no change in cleanup time, and therefore pertain to either hydraulic optimization or transport optimization:

- Scenario 1: 33% reduction in total pumping rate with no change in number of wells
- Scenario 2: 33% reduction in total pumping rate with 33% increase in number of wells

Unlike hydraulic optimization, transport optimization can be used to estimate the change in concentrations and/or cleanup time. Thus, additional alternative scenarios that pertain only to transport optimization can be considered that include potential reduction in cleanup time:

- Scenario 2a: 10% reduction in cleanup time based on Scenario 2
- Scenario 2b: 20% reduction in cleanup time based on Scenario 2
- Scenario 2c: 30% reduction in cleanup time based on Scenario 2

These alternative scenarios are summarized in Tables 3-1 and 3-2.

Table 3-1. Hydraulic Optimization Scenarios

	Pumping Rate	**Number of Wells**	**Reduction in Cleanup Time**
Baseline	No change	No change	no change
Scenario 1*	- 33%	No change	no change
Scenario 2	- 33%	+ 33%	no change

**maximum potential cost savings for hydraulic optimization expected from this scenario*

Table 3-2. Transport Optimization Scenarios (Initial Screening)

	Pumping Rate	**Number of Wells**	**Reduction in Cleanup Time**
Baseline	no change	no change	no change
Scenario 1	- 33%	no change	no change
Scenario 2	- 33%	+ 33%	no change
Scenario 2a	- 33%	+ 33%	-10%
Scenario 2b	- 33%	+ 33%	-20%
Scenario 2c*	- 33%	+ 33%	-30%

**maximum potential cost savings for transport optimization expected from this scenario*

The results from these scenarios are used to classify the sites into Tiers (defined within the screening methodology discussed in Appendix G) regarding potential benefits that

might be realized by performing an optimization analysis. The pre-optimization screening methodology can be used for both existing and planned systems.

Three sites were selected for the transport optimization demonstration:

- Umatilla Chemical Depot, Hermiston, Oregon (“Umatilla”)
- Tooele Army Depot, Tooele, Utah (“Tooele”)
- Former Blaine Naval Ammunition Depot, Hastings, Nebraska (“Blaine”)

Umatilla and Tooele have existing P&T systems in operation, and Blaine is in the design stage for a planned P&T system. Background for each site, plus details regarding the selection of each site, are presented below.

3.1.1. Umatilla Chemical Depot (“Umatilla”)

3.1.1.1. Site History

Umatilla is a 19,728-acre military reservation established in 1941 as an ordnance depot for storage and handling of munitions. The facility is located in northeastern Oregon straddling the border of the Umatilla and Morrow counties, three miles south of the Columbia River and six miles west of Hermiston, Oregon (Figure 3-1). The original mission of the Installation included the storage, renovation and demilitarizing of conventional munitions and storage of chemical munitions. In 1994, as a result of the Base Realignment and Closure (BRAC) Act, the depot's mission was changed to storing chemical munitions until their destruction under the Chemical Stockpile Disposal Program, and site remediation.

From the 1950s until 1965, the depot operated an onsite explosives washout plant. The plant processed munitions to remove and recover explosives using a pressurized hot water system. The wash water from the plant was disposed in two unlined lagoons, located northwest of the plant, where wash water infiltrated into the soil. During the 15 years of operation of the washout plant, an estimated 85 million gallons of wash water were discharged to the lagoons. Although lagoon sludge was removed regularly during operation of the plant, explosives contained in the wash water migrated into the soil and groundwater at the site. The groundwater table is encountered approximately 47 feet below the lagoons.

Two of the most common contaminants in groundwater are RDX (Hexahydro-1,3,5-trinitro-1,3,5-triazine, and commonly referred to as Royal Demolition Explosive) and TNT (2,4,6-Trinitrotoluene). These constituents are used as indicator parameters because they are found at high concentrations relative to other parameters.

Because of the soil and groundwater contamination of the lagoons, the site was placed on EPA’s National Priorities List (NPL) in 1984. The Army initiated a Remedial Investigation (RI) of the lagoons in 1987. Subsequently, a Human Health Baseline Risk

Assessment and a Feasibility Study (FS) were conducted. These evaluations were conducted to define remediation goals and criteria and to identify, evaluate, and provide the basis for selection of remedial alternatives for mitigating explosives contamination. The site was divided into Soils and Groundwater Operable Units.

Upon review of the RI/FS, the US Army, US Environmental Protection Agency (EPA), and the Oregon Department of Environmental Quality selected a cleanup plan for the groundwater operable unit. As described in the Record of Decision (USACE 1994), the selected alternative includes the following major components:

- Pumping groundwater from extraction wells over an estimated 10 to 30 year period

- Treating extracted groundwater with granular activated carbon (GAC) to remove contaminants

- In-situ flushing of subsurface soils beneath the lagoons with all or part of the treated groundwater for an estimated period of one year

- Reinfiltration of the treated groundwater outside the contaminant plume

- Monitoring of groundwater contamination to determine the effectiveness of the remedial action and to determine when groundwater cleanup levels have been attained

- Institutional controls on the contaminated groundwater to prevent its use until cleanup levels are met

Remediation of the groundwater is scheduled to continue until the concentration of explosives in the aquifer meets cleanup levels. The cleanup level for RDX is 2.1µg/l and for TNT is 2.8 µg/l.

3.1.1.2. Selection Criteria

Based on pre-optimization site screening, Umatilla met the following criteria:

- O&M costs are approximately $430K/year, which is greater than the screening criteria of 100K/year or greater

- System flowrate is 1300 gpm, which is greater than screening criteria of 50 gpm or greater

- Estimated cleanup time is 10 to 30 years, which is greater than the screening criteria of 5 years or greater

- Up-to-date flow and transport models that are considered reasonable to apply for design purposes exist for the site

- Site managers expressed a willingness to consider implementing recommendations that might arise from the optimization results

Using the screening methodology developed for this project (Appendix G), potential cost savings from application of optimization technology were calculated based on site-specific values provided by the installation and optimization screening scenarios (Table 3-1 and Table 3-2). The summary of potential cost savings is listed in Table 3-3 and the detailed cost calculations are included in Appendix G.

Table 3-3. Screening Tool Estimated Cost Savings(*) for Umatilla

Expected Duration	20 years	
CURRENT SYSTEM FORECASTED COST (NPV)	$5,613,603	
Hydraulic Optimization (Life-Cycle)		
▪ Maximum potential cost savings		$415,486
Transport Optimization (Life-Cycle)		
▪ Maximum potential cost savings, no reduction in cleanup time		$362,986
▪ Maximum potential cost savings, 10% reduction in cleanup time		$549,752
▪ Maximum potential cost savings, 20% reduction in cleanup time		$905,637
▪ Maximum potential cost savings, 30% reduction in cleanup time		$1,298,000

**These are "pre-optimization" estimates, not actual optimization results*

The pre-optimization screening results suggest that Umatilla could potentially benefit from both hydraulic optimization and transport optimization. Note that the site-specific values used for pre-optimization screening were based on "rough estimates" provided by the installation, while more rigorous data were compiled for the actual development of the optimization formulations (described later).

3.1.2. Tooele Army Depot ("Tooele")

3.1.2.1. Site History

Tooele was established in 1942 to provide storage, maintenance and demilitarization of troop support equipment, especially wheeled vehicles and conventional weapons. The site is illustrated on Figure 3-2. From 1942-1966, large quantities of hazardous materials

were used and generated from these operations in the industrial area. During this time period, the waste chemicals were piped through the industrial complex into a set of four unlined drainage ditches. These ditches ended at a set of natural depressions that were used as evaporation (and infiltration) ponds. These ponds have been called the Old Industrial Waste Lagoon (Old IWL). In 1966, a collector ditch was constructed to intercept the four existing ditches. This interceptor ditch ran north approximately 1.5 miles to an abandoned gravel pit, called the Industrial Wastewater Lagoon (IWL), which was used as an evaporation pond until its closure in 1988 when an industrial wastewater plant was brought on line. The primary contaminant of concern is TCE (Trichloroethylene), which was used as a solvent in the repair operations of military equipment.

In 1983, the Army began investigating sources of contamination contributing to a plume of TCE (the "Main Plume") that originated in the southeast portion of the Industrial Area and extends approximately 3.3 miles to the northwest. This plume was believed to have originated in the wastewater discharge through the unlined and the evaporation ponds. A groundwater pump and treat system was put in place to treat this Main Plume and prevent TCE concentrations greater than MCLs from crossing the property boundary. By the mid-1990's however it became apparent that there was contamination within the Main Plume that could not have originated in the IWL system and must therefore have originated at other sources within the industrial area or perhaps in the Defense Reutilization ad Marketing Office (DRMO) yard. Therefore, The Main Plume originates from several source areas within the industrial area and the IWL.

More recently, an additional plume (the "Northeast Plume") has been identified. The Northeast Plume originated from a recently identified point source in the industrial area, the oil/water separator at Building 679. The Northeast Plume extends beyond the property boundary, and the offsite extent is not fully characterized.

A recent Independent Technical Review (ITR), Final Draft dated December 2000, suggests that a risk-based approach be implemented. According to the ITR, the reissued Postclosure Permit (the principal legal driver for the site) will allow for the application of alternate concentration limits (ACL) via petition. Also according to the ITR, the Utah RCRA Regulations at R315, also known as "the Risk Rule" upon which the Postclosure Permit is based, will also be legally applicable requirements for remediation.

The ITR recommends that, for the Main Plume, the IWL and the industrial area should be considered one waste management area with the circumscribing line as the Point of Compliance (POC), and the downgradient property boundary considered as the Point of Exposure (POE). Using this approach, an Alternate Concentration Limit (ACL) is determined by establishing a contaminant concentration at the POC that will attain a concentration at the POE that is protective of human health and the environment taking into consideration the attenuation of contaminants between the POC and the POE. For the IWL/Industrial waste management area, the ACL would be the concentration of TCE at the POC that will result in a concentration of 5 ug/l of TCE at the POE.

3.1.2.2. Selection Criteria

Based on pre-optimization site screening, Tooele met the following criteria:

- O&M costs are over $1M/year, greater than screening criteria of $100K/year or more

- Current system flowrate is over 5000 gpm, greater than the screening criteria of 50 gpm or more

- Estimated cleanup time is uncertain, but is greater than the screening criteria of 5 years or more

- Up-to-date flow and transport models that are considered reasonable to apply for design purposes exist for the site

- Site managers expressed a willingness to consider implementing recommendations that might arise from the optimization results

Using the screening methodology developed for this project (Appendix G), potential cost savings from application of optimization technology were calculated based on site-specific values provided by the installation and optimization screening scenarios (Table 3-1 and Table 3-2). The summary of potential cost savings is listed in Table 3-4 and the detailed cost calculations are included in Appendix G.

Table 3-4. Screening Tool Estimated Cost Savings(*) for Tooele

Assumed Duration	20 years	
CURRENT SYSTEM FORECASTED COST (NPV)	$23,684,431	
Hydraulic Optimization (Life-Cycle)		
▪ Maximum potential cost savings		$3,379,423
Transport Optimization (Life-Cycle)		
▪ Maximum potential cost savings, no reduction in cleanup time		$3,329,423
▪ Maximum potential cost savings, 10% reduction in cleanup time		$2,781,459
▪ Maximum potential cost savings, 20% reduction in cleanup time		$4,161,829
▪ Maximum potential cost savings, 30% reduction in cleanup time		$5,683,687

**These are "pre-optimization" estimates, not actual optimization results*

The pre-optimization screening results suggest that Tooele could potentially benefit from both hydraulic optimization and transport optimization. Note that the site-specific values used for pre-optimization screening were based on "rough estimates" provided by the installation during Phase I, while more rigorous data were compiled for the actual development of the optimization formulations during Phase II.

3.1.3. Former Blaine Naval Ammunition Depot ("Blaine")

3.1.3.1. Site History

Blaine consists of 48,800 acres located immediately east of Hastings, Nebraska in eastern Adams County and western Clay County. The site is located 25 miles south of Grand Island, Nebraska and 105 miles west of Lincoln, Nebraska (Figure 3-3).

Blaine was built in the early 1940s as an active "load, assemble, and pack" ammunition facility during World War II and the Korean Conflict. Blaine was responsible for producing nearly one-half of the ordnance used by the Navy during WWII. During the World War II, the Korean Conflict, and the subsequent decommissioning process (1958-1967), waste materials were generated through discharge of wastewater to surface impoundments and natural drainage areas of the facility, and disposal of solid waste and explosives.

Beginning in the mid-1960s, large tracts of the former depot were either sold to various individuals, businesses, and municipalities or transferred to other governmental agencies. Much of the region's economy is based on agriculture. With sale and transfer of the land to the U.S. Department of Agriculture (USDA) and area farmers, over 100 irrigation wells have been installed on the former depot.

As a result of findings of groundwater contamination at Blaine in the mid-1980s, the EPA included portions of the former depot as part of the Hastings Groundwater Contamination Site (HGCS), a regional area of groundwater contamination in south-central Nebraska. The HGCS was added to EPA's National Priorities List (NPL) in 1986.

Five operable units (OUs) have been established for restoration of Blaine:

- OU4 consists of shallow soil (less than 10 feet in depth) at the Hastings East Industrial Park (HEIP)
- OU8 consists of vadose zone soil that separates OU4 and groundwater at the HEIP
- OU14 is groundwater which typically encountered at a depth of approximately 95 to 115 feet

- OU16 consists of three production areas of the former depot: the Explosives Disposal Area (EDA), the Naval Yard Dump (YD), and the Bomb and Mine Complex (BMC)

- OU15 is comprised of those remaining areas of Blaine that were not included as part of the other Operable Units.

Groundwater was first characterized during RI/FS activities from 1987 to 1990. A Supplemental RI of the Hastings East Industrial Park (HEIP) was conducted in 1990/1991 that included additional characterization of groundwater contamination. The data from the RI annual groundwater program, and the 1999 groundwater sampling event show that the VOC plumes encompass nearly six and one-half square miles. Additionally, groundwater contamination from explosives extends over an area of approximately three square miles and is commingled with the VOC plume(s) in several areas.

3.1.3.2. Selection Criteria

Blaine differs from the other two sites in that the P&T system is planned but does not yet exist. The ESTCP project team felt that demonstrating the application of transport optimization during the final design stage of a system might be of interest as part of the overall demonstration project. Based on pre-optimization site screening, Blaine met the following criteria:

- Designed O&M costs are approximately $2M/year, greater than the screening criteria of $100K/year or more

- Designed system flowrate is approximately 4000 to 5000 gpm, greater than screening criteria of 50 gpm

- Estimated cleanup time is 50 to 80 years, greater than the screening criteria of 5 years or more

- Up-to-date flow and transport models that are considered reasonable to apply for design purposes exist for the site

- Site managers expressed a willingness to consider implementing recommendations that might arise from the optimization results

Using the screening methodology developed for this project (Appendix G), potential cost savings from application of optimization technology were calculated based on site-specific values provided by the installation and optimization screening scenarios (Table 3-1 and Table 3-2). The summary of potential cost savings is listed in Table 3-5 and the detailed cost calculations are included in Appendix G.

Table 3-5. Screening Tool Estimated Cost Savings(*) for Blaine

Expected Duration	50 years	
CURRENT SYSTEM FORECASTED COST (NPV)	$49,083,815	
Hydraulic Optimization (Life-Cycle)		
▪ Maximum potential cost savings		$11,488,043
Transport Optimization (Life-Cycle)		
▪ Maximum potential cost savings, no reduction in cleanup time		$11,435,543
▪ Maximum potential cost savings, 10% reduction in cleanup time		$10,507,852
▪ Maximum potential cost savings, 20% reduction in cleanup time		$12,268,370
▪ Maximum potential cost savings, 30% reduction in cleanup time		$14,359,313

**These are "pre-optimization" estimates, not actual optimization results*

The pre-optimization screening results suggest that Blaine could potentially benefit from both hydraulic optimization and transport optimization. Note that the site-specific values used for pre-optimization screening were based on "rough estimates" provided by the installation, while more rigorous data were compiled for the actual development of the optimization formulations.

3.2 Site/Facility Characteristics

3.2.1. Umatilla

3.2.1.1. Site Hydrogeology

The hydrogeology for Umatilla consists of an alluvial aquifer overlying silt and weathered basalt. The hydraulic conductivity values in the alluvial aquifer are heterogeneous, ranging from approximately 1 ft/day to approximately 5000 ft/day. The hydraulic conductivity of the silt and weather basalt is much lower (approximately 1 ft/day to 6 ft/day). Net recharge from precipitation is very low (approximately 0.5 inches per year).

3.2.1.2. Plume Definition

RDX and TNT are contaminants of concern (COCs) for this site. Figure 3-4 illustrates the concentrations and extent of impacts of the RDX and TNT plumes prior to operation of the groundwater P&T system. This figure also illustrates the locations of key components of the P&T system (discussed in more detail later). The figure illustrates that the RDX plume is much bigger in area than the TNT plume. This is because TNT is

more strongly sorbed to the aquifer materials, and therefore its movement is retarded relative to groundwater velocity to a much greater extent than RDX.

3.2.1.3. Existing Remediation System

A groundwater P&T system was implemented in January 1997. Design of the groundwater treatment system was based in part on the results of groundwater modeling studies. The remedial design configuration is shown in Figure 3-4.

The current P&T system has three active extraction wells (EW-1, EW-3, and EW-4), and three active infiltration basins (IF1, IF2, and IF3). The infiltration basins are located around the perimeter of the pre-pumping RDX plume, and were intended to augment hydraulic control. Well EW-2 was drilled approximately 100 feet northwest of EW-4, but a pump and associated piping were never installed. An additional infiltration basin, IFL, is the location of a former industrial lagoon (i.e., a source area of the contamination), and it was used as in infiltration basin in the early stages of the remedy to promote in-situ flushing of the unsaturated zone. However, use of that location for infiltration was terminated due to concerns that it could cause unwanted spreading of the TNT plume.

The contaminated groundwater is extracted from the wells and then sent to GAC units, which remove the contaminants. The treated water is discharged to the infiltration basins. The current GAC capacity is 1300gpm. The system has operated routinely, with the exception of an extended period of shutdown for treatment system adjustment during the first quarter of operation, intermittent power outages, and periodic treatment plant shutdown during GAC replacement events which cause the system to be down approximately 10% of the time. The current extraction rates and recharge rates (as implemented in the current site groundwater model) are listed in Table 3-6.

Table 3-6. Modeled Pumping Rates, Current System*

Wells / Recharge Basins	Rate (gpm)
EW-1	128.227
EW-2	0
EW-3	105.046
EW-4	887.24
IF1	232.80
IF2	405.27
IF3	482.40

**These rates are 10% lower than actual average rates, to account for system down-time.*

The annual O&M cost for the current system is approximately $430K/year, apportioned as follows:

- $237K/yr as Labor
- $103K/yr as Materials
- $ 62K/yr as Analytical
- $ 27K/yr as Electric

Approximately 1.27 billion gallons of contaminated groundwater was extracted, treated and recharged to the aquifer by 15 July 1999. The mass removed from the aquifer during this time period was estimated to be 3,000 kg for RDX and 400 kg for TNT.

3.2.1.4. Groundwater Flow and Transport Models

The site had previously developed three-dimensional flow and transport models, with the codes MODFLOW and MT3DMS. The model, re-calibrated in May 2000, has 125 rows, 132 columns, and 5 layers, with variable grid spacing of 24.8ft – 647.9ft along the rows and 21.6ft – 660.7ft along the columns. Model layers are assigned as follows:

- Layer 1: alluvial aquifer, unconfined
- Layer 2: silt and weathered basalt, convertible (confined/unconfined)
- Layer 3: silt and weathered basalt, convertible (confined/unconfined)
- Layer 4: silt and weathered basalt, convertible (confined/unconfined)
- Layer 5: silt and weathered basalt, convertible (confined/unconfined)

The Installation only focuses on contaminant transport in layer 1 of the model, and requested that the optimization study conform to that approach.

The model units are in feet and years. The hydraulic conductivity values in layer 1 range from 375ft/yr to 1.8×10^{6}ft/yr and 375ft/yr to 2000ft/yr for layers 2-5. Net recharge is applied to the layer 1 at a rate of 0.0417ft/yr (0.5 in/yr). The boundary conditions are simulated as constant head along all the four edges of the model. Some modifications were made to the existing model for this demonstration project:

- Transport solution package was changed from method of characteristics to finite-difference to reduce the simulation time from 10 hours to about 10 minutes (model accuracy was not affected)

- Model time discretization was modified to incorporate four 5-year stress periods to match the management periods defined in the optimization formulations

- The initial time in the model for the transport optimization was set as January 1, 2003, to account for a realistic time when modifications to the existing system could be implemented (the optimization study was completed for this site approximately 1.5 years prior to that date)

The computational time for a flow and transport simulation run with the model, for the full 20-year simulation period, is approximately 10 minutes on a PC with a Pentium III 1-Ghz CPU.

3.2.2. Tooele

3.2.2.1. Site Hydrogeology

The facility is located in Tooele Valley in Utah, several miles south of the Great Salt Lake. The aquifer of concern generally consists of alluvial deposits. However, there is an uplifted bedrock block at the site where groundwater is forced to flow from the alluvial deposits into fractured and weathered rock (bedrock), and then back into alluvial deposits.

The unconsolidated alluvial deposits are coarse grained, consisting of poorly sorted clayey and silty sand, gravel, and cobbles eroded from surrounding mountain ranges. There are several fine-grained layers assumed to be extensive but discontinuous, and these fine-grained layers cause vertical head differences between adjacent water-bearing zones. Bedrock that underlies these alluvial deposits is as much as 400 to 700 feet deep. However, in the vicinity of the uplifted bedrock block, depth to bedrock is much more shallow, and in some locations the bedrock is exposed at the surface.

The hydraulic conductivity of the alluvium varies from approximately 70 to 400 ft/day in the areas upgradient and downgradient of the bedrock. In the bedrock area, hydraulic conductivity ranges from approximately 0.04 ft/day to 0.96 ft/day for the fractured bedrock. In the displaced sediment area adjacent to the fractured bedrock, the hydraulic conductivity is approximately 1.3 ft/day.

Groundwater flow trends in a northwest direction. Uplifted, fractured bedrock in the central area is a controlling hydrogeological feature at the Tooele site (Figure 3-5). In general, the site can be divided into three separate hydrogeologic regimes, 1) the fractured bedrock and adjoining low conductive alluvium in the central area; 2) the highly transmissive alluvium in the northern downgradient part; and 3) the shallow alluvium at the southern upgradient end of the site. The uplifted bedrock block and adjoining low hydraulic conductivity alluvium are the hydraulically controlling features of the study area due to the steep gradients they cause. The uplifted bedrock block strikes roughly east-northeast and dips north–northwest. On the local scale the bedrock block exhibits strongly heterogeneous hydrogeology typical of fractured flow environments. Flow through the bedrock block consists of a steep gradient when entering the bedrock, a flatter gradient through the bedrock core and a steep gradient when exiting the bedrock.

3.2.2.2. Plume Definition

The specific plume evaluated in this study, the Main Plume, originates from an industrial area in the southeastern corner of the facility, where former operations (since 1942)

included handling, use, and storage of TCE and other organic chemicals. Groundwater monitoring indicates that the primary contaminant is TCE, although other organic contaminants have been detected. TCE concentrations in the shallow portion of the aquifer are presented on Figure 3-6. Concentrations are significantly lower in the deeper portions of the aquifer than in shallow portions of the aquifer. Also, the extents of the shallow and deep plumes do not directly align, indicating a complex pattern of contaminant sources and groundwater flow. Continuing sources of dissolved contamination are believed to exist (see Figure 3-5).

3.2.2.3. Existing Remediation System

A pump-and-treat system has been operating since 1993. The system consists of 16 extraction wells (15 are operating and one is not operating) and 13 injection wells (see Figure 3-6 for well locations). An air-stripping plant, located in the center of the plume, is capable of treating 8000 gpm of water. It consists of two blowers operated in parallel, each capable of treating 4000 gpm. Sodium hexametaphosphate is added to the water prior to treatment, to prevent fouling of the air stripping equipment and the injection wells. Treated water is discharged via gravity to the injection wells.

Based on the well locations and previous plume delineations, the original design was for cleanup. At the time the system was installed, the source area was assumed to be north of the industrial area (near a former industrial waste lagoon). Subsequently, it was determined that the source area extended far to the south (in the industrial area). As a result, the current system essentially functions as a containment system (there are no extraction wells in the area of greatest contaminant concentration).

Historically, the target containment zone has been defined by the 5-ppb TCE contour. Given the current well locations and continuing sources, anticipated cleanup time is “a very long time”. However, a revised (i.e., smaller) target containment zone is now being considered, based on risks to potential receptors. A revised target containment zone might correspond to the 20-ppb or 50 ppb-TCE contour.

3.2.2.4. Groundwater Flow and Transport Models

A three-dimensional, steady-state MODFLOW model was originally constructed in 1993 (subsequent to the design of the original system), and has been recalibrated on several occasions (to both non-pumping and pumping conditions). The current model, recalibrated in spring 2001, has 4 layers, 165 rows, and 99 columns. Cell size is 200 ft by 200 ft. Model layers were developed to account for different well screen intervals, and are assigned as follows:

- Layer 1: 0 to 150 ft below water table
- Layer 2: 100 ft thick
- Layer 3: 150 ft thick
- Layer 4: 300 ft thick

Boundaries include general head conditions up- and down-gradient, and no flow at the sides and the bottom.

The groundwater solute transport is simulated with MT3DMS. Some modifications were made to the existing model for this demonstration project:

- Model time discretization was modified to have seven 3-year stress periods to match the management periods defined in the optimization formulations

- The initial time in the model for the transport optimization was set as January 1, 2003, to account for a realistic time when modifications to the existing system might be implemented (the optimization study was completed for this site approximately 1 year prior to that date)

- The initial TCE plume was generated for the optimization study based on model simulated concentrations on 12/31/2002, which were then mathematically conditioned using the most recent concentration measurements at several locations

Many test runs were performed prior to optimization period to prove the existence of feasible solutions for Formulations 1 & 2. Each flow and transport simulation run takes less than 10 minutes on a PC with a Pentium III 1-Ghz CPU.

3.2.3. Blaine

3.2.3.1. Site Hydrogeology

Groundwater is encountered in the study area approximately 100 feet below ground surface. The three saturated hydrogeologic units of primary interest of this study are, in descending order:

- The unconfined aquifer
- The upper confining layer
- The semi-confined aquifer

The unconfined aquifer consists of sand and gravel and clayey or silty sand. It is relatively thin, with a thickness of about 10 to 15 feet. The upper confining layer consists of silty clay, clayey silt and clayey sand. Although this confining layer is present under most of the region, it is absent or discontinuous in a significant part of the study area. The thickness of the upper confining layer is typically 1 to 3 feet, but is as great as 20 feet northeast of the HEIP. In areas where the clay layer is discontinuous, particularly in the middle portion of the model area, the thickness of the “clay layer” generally ranges from 0 to 1 foot.

The semi-confined aquifer has a thickness of 100 to 150 feet in the study area, and consists of sand and gravel with discontinuous layers of silty clay and clayey sand. The semi-confined aquifer is the major water supply aquifer in the region, and supports municipal, industrial, and particularly, irrigation needs.

In the model, hydraulic conductivity ranges from 10 to 80 ft/day in the unconfined aquifer, 0.002 to 0.5 ft/day for the confining layer, and 150 – 250 ft/day for the semi-confined aquifer. Groundwater recharge in the area of interest was simulated as spatially variable to reflect the different rates in non-irrigation zones and irrigation zones. The estimated net recharge for non-irrigated areas equals 1.8 in/yr and the estimated rate for irrigated areas equals 2.9 in/yr.

The groundwater flow directions for both the unconfined and semi-confined aquifers are predominantly to the east and southeast during non-irrigation seasons with an average hydraulic gradient of 0.001. During irrigation season, which lasts about two and half months, heavy pumping from extensive irrigation wells dramatically alters the groundwater flow direction.

3.2.3.2. Plume Definition

Groundwater contamination at Blaine is primarily due to chemical spills and/or discharge of wastewater to surface impoundments, wastewater systems, and natural drainages, mainly in production areas. The contaminants of concern in groundwater are VOCs and explosives.

Recent groundwater analyses suggest that the VOC plumes encompass nearly six square miles. Although information on the vertical distribution of contaminants in the semi-confined aquifer is limited in the middle and lower portions of the aquifer, groundwater analyses from the deep wells demonstrate that contamination is absent in the lowest portion of the unconsolidated aquifer. Explosives-related groundwater contamination extends over an area of approximately three square miles and is commingled with the VOC plumes in several areas (Figure 3-7).

The RI and the annual groundwater sampling results identified seven source areas for VOCs with plumes commingling at six of the source areas and one primary source for explosives. Extensive remediation of source areas by soil vapor extraction (SVE) or soil excavation is being implemented or has been completed.

3.2.3.3. Planned Remediation System

There is no existing groundwater extraction remediation system at Blaine. This site is in the final design stages, based on a Feasibility Study performed in August 2000. The Feasibility Study dated in August 2000 focused on three remediation alternatives:

- Hydraulic Containment

- Aggressive Remediation
- Focused Remediation

The Hydraulic Containment alternative consists of groundwater extraction intended primarily to hydraulically contain the existing contaminant plumes. This scenario includes 12 deep extraction wells and 5 shallow extraction wells. The total extraction rate is 4050 gpm from the deep wells and 18 gpm from the shallow wells. The estimated duration is about 60 years for all the contaminants to reach the target cleanup levels.

The Aggressive Remediation alternative consists of groundwater extraction throughout the impacted areas. This scenario includes 24 deep extraction wells and 10 shallow extraction wells. The total pumping rate is 4140 gpm from the deep wells and 27 gpm from the shallow wells. The estimated duration is 50 years for all the contaminants to reach the target cleanup levels with no offsite migration.

The Focused Remediation alternative consists of groundwater extraction in selected areas of higher concentrations. This scenario includes 12 deep extraction wells and 10 shallow extraction wells. The total pumping rate is 2458 gpm from the deep wells and 44 gpm from the shallow wells. The maximum duration of operation for the groundwater extraction and treatment system is estimated to be 30 years. However, a period of 150 years is estimated for all the contaminants to reach the target cleanup levels with no offsite migration.

3.2.3.4. Groundwater Flow and Transport Models

Groundwater flow is simulated with the MODFLOW code. The model grid covers 134 square miles. Variable cell dimensions range from 400 ft by 400 ft in the center of the model, to 2000 ft by 2000 ft near the model edges. There are six model layers:

- Layer 1 is the unconfined aquifer
- Layer 2 is the upper confining layer
- Layers 3-6 are the semi-confined aquifer, split evenly into 4 layers with the equal thickness and same properties

The model boundary conditions for all four sides of the model domain were specified as general head boundaries. General head boundary conditions allow exchange of flow across the model boundaries in response to hydraulic stresses applied to the flow system. The groundwater flow model was calibrated to both steady-state and transient conditions, and included particle tracking to calibrate based on historical plume shape and plume length. Calibrated horizontal hydraulic conductivities range from 10 to 80 ft/day in the unconfined aquifer, and 150 to 250 ft/day in the semi-confined aquifer. Hydraulic conductivity of the upper confining bed is much lower, ranging 0.002 to 0.5 ft/day.

Groundwater contaminant transport is simulated with MT3DMS. In the FS, the following six parameters were simulated:

- TCE (VOC)
- PCE (VOC)
- 1,1,1-TCA ("TCA") (VOC)
- 1,1-DCE ("DCE") (VOC)
- TNT (Explosive)
- RDX (Explosive)

The optimization project is restricted to simulation of two parameters. Site managers selected TCE and TNT as the parameters most important to remedial design. However, site managers also indicated a preference to not ignore the other parameters. Therefore, an approach (discussed in formulation document, see Appendix F) was developed to incorporate the distribution of the other constituents.

For all three optimization formulations, surface disposal is only considered for discharge of treated groundwater outside of the modeled area, as requested by the site managers. Thus, treated extracted groundwater does not influence the groundwater model inputs. A capital discharge piping cost and a variable discharge cost based on discharge rate are included in the cost objective function for Formulations 1 and 2.

Some modifications were made to the existing model for this demonstration project:

- The original model, which consisted of 30 one-year models run sequentially (because of dry cell issues) was converted to one 30-year model

- The MODFLOW96 code was modified to compute a head at cells where water levels fell below bottom elevation, rather than removing such cells from the simulation

- The MODFLOW drain package was used to simulate the low-flow wells in model layer 1; flow rates at these wells were fixed during the optimization to prevent dry cells that might be caused by too much pumping in an unconfined aquifer

- TCE, PCE, TCA, DCE, and RDX were all simulated as one TCE plume for the optimization simulation

- The initial time for the transport optimization in the model was set as September, 2003 to account for a realistic time when remediation system design might be implemented (the optimization study was completed for this site approximately1 year prior to that date)

Many test runs were performed prior to optimization period to prove the existence of feasible solutions for formulations. The flow and transport model takes over 2 hours per simulation on a Pentium III 1-Ghz PC.

4. Demonstration Approach

4.1 Performance Objectives

The performance objective of the overall project is to demonstrate the cost benefit of applying transport optimization codes, by addressing the following questions:

- Do the results obtained from these optimization software packages (e.g. recommended optimal pump and treat scenarios) differ substantially from the optimal solutions determined by traditional “trial-and-error” optimization methods?

- Do the results obtained from these optimization software packages warrant the additional effort and costs when compared to traditional “trial-and-error” optimization methods?

Three site-specific optimization formulations were developed for each site, based on interaction with the installation. Some of the formulations included non-cleanup objectives, such as minimizing the mass remaining in the aquifer, minimizing the total pumping rate, etc. Each of three modeling groups then independently determined the optimal solution for each of the formulations, with no further discussions with the installation during the optimization periods. Two of the modeling groups used their own independently developed transport optimization software, and the other group used a traditional “trial-and-error” optimization method. Thus, the results from two separate transport optimization software programs can be compared to each other, and to the recommendations from an experimental control (the trial and error group).

A third-party expert (Dr. Barbara Minsker) was added to the project team during the beginning of Phase 2 to evaluate the performance objective of the overall project, based on the results from the three demonstration sites. This evaluation considers the improvement in objective function value resulting from the application of the transport optimization algorithms, specific approach and algorithms employed, associated parameters used in the optimization algorithms, and any additional effort, cost, and/or expertise required to implement the optimization algorithms, plus any additional benefits associated with the application of transport optimization algorithms.

In addition to the performance objectives for the overall project, each demonstration site had site-specific objectives represented by the objective function associated with each of the three mathematical formulations posed for the site. These site-specific objectives are summarized in Table 4-1. The system durations listed in Table 4-1 were developed as part of the optimization formulations, based on consultation with the site installations or site managers.

Table 4-1. Site-Specific Objectives Represented By Objective Function

Site	Site-Specific Objective
UMATILLA	Formulation 1 and 2: Minimize system life-cycle cost Formulation 3: Minimize total mass remaining after 20 years
TOOELE	Formulations 1 to 3: Minimize system cost over 21 years
BLAINE	Formulation 1 and 2: Minimize system life-cycle cost Formulation 3: Minimize maximum total pumping rate in any management period

4.2 Setup and Operation

4.2.1. Overall Project Operation

Once sites were selected (Phase 1), the following activities were associated with performing the transport optimization for each site (Phase 2):

- An initial draft of potential optimization formulations was developed by the Management Team, based on a site visit (performed in Phase 1) and subsequent phone conversations and/or emails with the installation

- Feedback on the initial draft optimization formulations was provided by the installation, including details on cost coefficients and/or constraint values

- To limit the scope of this demonstration project, the simulation models were modified as necessary to require no more than 2 hours of computational time and to include no more than 2 constituents simulated

- The formulations were finalized and distributed to each modeling group by GeoTrans, including a feasible solution if one had been determined during the formulation process, and a FORTRAN post-processor for determining the objective function value and status of the constraints for any specific combination of well rates simulated with the transport model (the FORTRAN code allows for third-party verification of results)

- Optimization for each of the three formulations for the site was performed over a period of approximately four months, during which time the three modeling groups (two transport optimization groups and one trial and error group) were not allowed to discuss their progress with each other (bi-weekly progress reports were submitted by each group to the US Navy)

- Each modeling group submitted a report describing the results for each site after the optimization period (Appendices D – F)

- After optimization was complete, the Management Team and modeling groups met to present and interpret results, with a subsequent presentation of results to the installation by a subset of the Management Team

A summary of these activities for each of the three demonstration sites, including the approximate duration, is presented in Table 4-2.

Table 4-2. Summary of Activities

Activity	Umatilla	Tooele	Blaine
Site Visit (Phase 1)	8/23/00	5/31/01	10/17/01
Develop Formulations	10/16/00 – 3/21/01	6/4/01 – 10/31/01	1/15/02 – 5/15/02
Optimization Period	3/22/01 – 7/16/01	11/1/01 – 2/28/02	5/17/02 – 9/17/02
Project Team Meeting to Present Results	10/18/01	3/20/02	9/19/02
Present Results to Installation	11/15/01	5/16/02	9/30/02
Follow-up with Installation	3/19/02	12/02	12/02

A summary of key aspects of the three formulations for each of the three demonstration sites is listed in Table 4-3. A brief description of the formulations for each site is presented in Section 4.2.3 to Section 4.2.5, respectively. The detailed formulations are presented in Appendices D to F.

Table 4-3. Formulation Summary (Key Aspects) f or the Three Demonstration Sites

<table>
<tr><th colspan="2">Site Name</th><th>Objective Function</th><th>Major Constraints</th></tr>
<tr><td rowspan="3">Umatilla</td><td>Form. 1</td><td>Minimize life-cycle cost until cleanup</td><td>1. Current treatment capacity
2. Cleanup of RDX and TNT < 20 yrs</td></tr>
<tr><td>Form. 2</td><td>Minimize life-cycle cost until cleanup</td><td>1. Increased treatment capacity
2. Cleanup of RDX and TNT < 20 yrs</td></tr>
<tr><td>Form. 3</td><td>Minimize total mass remaining in layer 1 after 20 yrs</td><td>1. Cleanup of RDX and TNT
2. Limit on # new wells and recharge basins</td></tr>
<tr><td>Tooele</td><td>Form. 1</td><td>Minimize total cost over 21 years</td><td>1. POE concentration limit for TCE at site boundary after 3 yrs</td></tr>
</table>

	Form. 2	Minimize total cost over 21 years	1. POE concentration limit for TCE at site boundary after 3 yrs 2. POC concentrations limits for TCE at specific locations/times within site boundary
	Form. 3	Minimize total cost over 21 years	1. POE/POC concentration limits 2. Declining source term 3. Cleanup (TCE < 50ppb) at most locations within 9 years
Blaine	Form. 1	Minimize life-cycle cost until cleanup	1. Plume containment 2. Cleanup of TCE and TNT < 30 yrs
	Form. 2	Min life-cycle cost until cleanup w/ 2400 gpm extracted water diverted	1. Plume containment 2. Cleanup of TCE and TNT < 30 yrs
	Form. 3	Min maximum total pumping	1. Plume containment 2. Limit on number of new wells

**Note: see Appendices D-F for detailed formulations for each site*

4.2.2. Optimization Approaches

The traditional trial-&-error method was used by GeoTrans to serve as a scientific control for the transport optimization groups. Two transport optimization modeling groups, Dr. Chunmiao Zheng of University of Alabama (UA) and Dr. Richard Peralta of Utah State University (USU), used their own independently developed simulation-optimization software for this study. These investigators were chosen based upon selective criteria that included availability of user-friendly optimization packages and prior field implementation of their optimization packages in a similar fashion to what was intended for this project, though the specific codes/algorithms they would apply for this project were their choice. The transport simulation-optimization packages used were:

- Dr. Zheng (UA): *Modular Groundwater Optimizer (MGO)*. The MGO code is implemented with genetic algorithm (GA), simulated annealing (SA), and tabu search (TS). MGO also includes options for integrating the response function approach with GA/SA/TS for greater computational efficiency (see *Zheng and Wang*, 2002).

- Dr. Peralta (USU): *Simulation/Optimization Modeling System (SOMOS)*. SOMOS includes genetic algorithm linked with tabu search (GA+TS), simulated annealing linked with tabu search (SA+TS), and artificial neural network (ANN). ANN is used as a fast-running simulator for state variables. SOMOS also includes response function options which have been used for many sites (SSOL, 2001 – 2003)

The MGO code was written in FORTRAN language and the executable program was compiled by Lahey FORTRAN 90 compiler (LF90) to run on personal computers

equipped with Intel-compatible Pentium processor or higher in the DOS boxes of Windows 95/98/NT/2000. More detailed information can be found in the MGO user manual.

The SOMOS code is written and compiled using Microsoft Visual C++ to run on personal computers equipped with Intel-compatible Pentium processor or higher. The most recent version runs under Windows NT/2000/XP. Detailed information is in the SOMOS user manual.

The user manuals for SOMOS and MGO also contain additional information on the algorithms, including suggestions for effective implementation. All of the algorithms used in this project are “heuristic” algorithms, meaning that they are not guaranteed to find the globally optimal solution but have usually been found in practice to identify what are believed to be near-globally optimal solutions. While some algorithms exist that can find guaranteed global optima, they can only be applied to certain types of problems (e.g., closed form, differentiable objective functions and constraints) and hence cannot be applied to the types of formulations considered in this project.

4.2.3. Formulation Summary: Umatilla

Three different transport optimization formulations, consisting of an objective function to be minimized and a set of constraints to be satisfied, were developed for Umatilla. These formulations are based on data from the system operated from 1997 to the present, and from input provided by the installation and the Army Corp of Engineers Seattle District (collectively referred to herein as “the Installation”). A detailed presentation of the formulations is presented in Appendix D. A brief summary is provided below.

The Installation expressed interest in achieving cleanup for both RDX and TNT at the lowest life-cycle cost. The current model indicates that a feasible solution exists for cleaning up both RDX and TNT within 20 years, and that was set as an upper bound on cleanup time. The Installation also expressed interest in determining the benefit of increasing the capacity of the treatment plant above the current capacity of 1300 gpm. The first two formulations address those interests. A third formulation was then constructed with a simpler objective function, minimizing mass remaining, to see if substantially different solutions would result.

A simple description of the formulations is as follows:

Formulation 1: Minimize the life-cycle cost (until cleanup of both RDX and TNT), subject to: 1) the current capacity of the treatment plant is held constant, 2) the cleanup of both RDX and TNT is within 20 years.

Formulation 2: same as Formulation 1, but allows the capacity of the treatment plant to increase to a maximum of 1950 gpm.

Formulation 3: Minimize the total mass remaining (RDX plus TNT) in layer 1 within 20 years.

Some additional details on each formulation are provided below (full details are presented in Appendix D).

Formulation 1

The cost function to be minimized combines the "Up-Front Costs" with the "Total of Annual Costs" over the time it takes to reach cleanup for both RDX and TNT, assuming a discount rate of 5%. The components of cost are:

MINIMIZE (CCW + CCB + FCL + FCE + VCE + VCG + VCS)

where

CCW:	Capital costs of new wells ($75,000 per well, $25,000 for EW-2)
CCB:	Capital costs of new recharge basins ($25,000 per basin)
FCL:	Fixed cost of labor ($237,000 per year)
FCE:	Fixed costs of electricity ($3,600/year)
VCE:	Variable electrical costs of operating wells (depends on pumping)
VCG:	Variable costs of changing GAC units (depends on influent conc.)
VCS:	Variable cost of sampling (depends on plume area)

Constraints include the following:

- The modeling period consists of four 5-year management periods (20 years total) beginning January 2003;
- Modifications to the system may only occur at the beginning of each management period;
- Cleanup, for both RDX and TNT, must be achieved within modeling period (by the end of year 20);
- The total modeled pumping rate, when adjusted for the average amount of uptime, cannot exceed 1300gpm, the current maximum treatment capacity of the plant;
- The extraction system must account for limits imposed by the hydrogeology of the site (limit of 400 gpm or 1000 gpm, depending on location, adjusted for system downtime);
- RDX and TNT concentration levels must not exceed their respective cleanup levels in locations beyond a specified area;
- The total pumping rate and total infiltration rate have to be balanced.

Formulation 2

The objective function is the same as for Formulation 1, except an addition term is added:

CCG: Capital cost of new GAC unit @ 325 gpm ($150,000 per unit)

Constraints are the same as for Formulation 1, except that treatment plant capacity could be increased in steps of 325 gpm, from the current capacity of 1300 gpm to a maximum capacity of 1950 gpm.

Formulation 3

The objective function is to minimize the total mass remaining (RDX plus TNT) in layer 1 at the end of 20 years. The constraints are the same as Formulation 1, except the maximum number of new wells cannot exceed 4, and the maximum number of new recharge basins cannot exceed 3.

4.2.4. Formulation Summary: Tooele

Three different transport optimization formulations, consisting of an objective function to be minimized and a set of constraints to be satisfied, were developed for Tooele. The Northeast Plume is not well-defined, and for the purpose of this study (based on a request from the installation), all formulations include a specified well in the Northeast Plume with 1500 gpm (implemented as 1425 gpm in the well package to account for downtime of 5%) to represent a general containment solution in that area. A detailed presentation of the formulations is presented in Appendix E. A brief summary is provided below.

Definitions specific to the formulations are:

POE-MP: "Point of Exposure – Main Plume": TCE concentrations cannot exceed 5 ug/L for TCE at the POE-MP in all model layers at the POE, which is located along a portion of the property boundary.

POC-MPx: "Point of Compliance – Main Plume": POC-MP1 is defined as the southern boundary of the displaced sediments. POC-MP2 is defined as the boundary along the upstream edge of the low permeability gouge surrounding the bedrock.

A simple description of the formulations is as follows:

Formulation 1: Minimize total cost over 21 years, subject to meeting specific concentration limits at the POE boundary.

Formulation 2: Same as formulation 1, but also meet aggressive concentration limits at the POC boundaries.

Formulation 3: Same as Formulation 2, but include a declining source term rather than a continuous source term for unremediated sources, and add additional cleanup constraints within the plume

Some additional details on each formulation are provided below (full details are presented in Appendix E).

Formulation 1

A cost function to be minimized was developed (in conjunction with the installation) that combines the "Up-Front Costs" with the "Total of Annual Costs" over a 21-year time frame, beginning January 2003, assuming a discount rate of 5%. The components of cost are:

MINIMIZE (CCE + CCI + FCO + VCE + VCS + VCC)

where

- CCE: Capital costs of new extraction wells ($307,000 per well)
- CCI: Capital costs of new injection wells (223,000 per well)
- FCO: Fixed cost of O&M ($525,000 per year)
- VCE: Variable electrical costs of operating wells (depends on # extraction wells)
- VCS: Variable costs of sampling (depends on plume area)
- VCC: Variable cost of chemicals (depends in flow rate)

Constraints include the following:

- The modeling period consists of seven 3-year management periods (21 years total) beginning January 2003;
- Modifications to the system may only occur at the beginning of each management period;
- The total modeled pumping rate, when adjusted for the average amount of uptime, cannot exceed 8000gpm, the current maximum treatment capacity of the plant;
- The POE constraint, i.e., 5ppb, has to be met in each layer at the end of the first three-year management period, and thereafter;
- The extraction and injection wells cannot exceed the rate limits;
- The total pumping rate and total reinjection rate have to be balanced.

Formulation 2

Same as Formulation 1, except includes additional constraints requiring concentration limits to be met at the POC (i.e., inside the plume):

- POC-MP1 must be 50% of the initial concentrations or < 20 ug/l at the end of the first management period (year 3), and thereafter; and
- POC-MP2 must be 50ppb at the end of the first management period (3 yrs), and 20ppb at the end of the third management period (9 yrs) and thereafter.

Formulation 3

This Formulation also includes a source term that declines over time, unlike the first two formulations (which have continuing sources at constant strength over time). The objective function is the same as formulations 1 and 2. The constraints are the same as Formulation 2, with the following additional constraints:

- Cleanup (defined as TCE <50ppb) for the Main Plume (except specifically excluded areas) must be met at the end of 9 years
- The maximum number of new extraction wells cannot exceed 4
- The maximum number of new injection wells cannot exceed 4

4.2.5. Formulation Summary: Blaine

Three different transport optimization formulations, consisting of an objective function to be minimized and a set of constraints to be satisfied, were developed for Blaine. The ESTCP project had a limit of only two parameters to be rigorously simulated in the optimization process, but the installation was concerned about six parameters, so an approach was developed to rigorously simulate TCE and TNT, and to incorporate the distribution of the other constituents in those simulations. A detailed presentation of the formulations (including this approach for multiple constituents) is presented in Appendix F. A brief summary is provided below.

A simple description of the formulations is as follows:

Formulation 1: Minimize life-cycle cost subject to: 1) the plumes cannot spread above cleanup levels beyond specified areas; 2) cleanup of both TCE and TNT must be within 30 years in model layers 3-6.

Formulation 2: same as Formulation 1 but assumes diversion of 2400 gpm of extracted water to a utility (i.e., that water does not require treatment and subsequent discharge)

Formulation 3: Minimize the maximum total remediation pumping rate in any management period over a 30-year simulation, such that the plumes do not spread above cleanup levels beyond specified areas.

Some additional details on each formulation are provided below (full details are presented in Appendix F).

Formulation 1

A cost function to be minimized was developed (in conjunction with the installation) that combines the "Up-Front Costs" with the "Total of Annual Costs" over the time it takes to reach cleanup for TCE and TNT in model layers 3-6, beginning September 2003, assuming a discount rate of 3.5%. The components of cost are:

MINIMIZE (CCE + CCT + CCD + FCM + FCS + VCE + VCT + VCD)

where

CCE: Capital cost of new extraction wells ($400,000/well)
CCT: Capital cost of treatment ($1,000/gpm)
CCD: Capital cost of discharge ($1,500/gpm)
FCM: Fixed cost of management ($115,000/yr)
FCS: Fixed cost of sampling ($300,000/yr)
VCE: Variable electrical cost of operating wells ($46/gpm/yr)
VCT: Variable cost of treatment ($283/gpm/yr)
VCD: Variable cost of discharge ($66/gpm/yr)

Constraints include the following:

- The modeling period consists of six 5-year management periods (30 years total) beginning September 2003
- Modifications to the system may only occur at the beginning of each management period
- Cleanup, for both TCE and TNT, must be achieved in model layers 3-6 within the modeling period (by the end of year 30)
- TCE and TNT concentration levels must not exceed their respective cleanup levels in locations beyond specified areas (i.e., containment must be achieved)

- Site managers used specific capacity assumptions to determine the limits on individual extraction well rates:

  - well screens one model layer: 350 gpm limit
  - well screens two model layers: 700 gpm limit
  - well screens three model layers: 1050 gpm limit

- Multi-aquifer wells must have equal rate in each model layer (since transmissivity is the same in model layers 3, 4, and 5)

- Some restricted areas are defined where no remediation wells are allowed

- Remediation wells are not allowed in the same model cells with irrigation wells to prevent excessive dewatering in irrigation wells and/or at remediation wells

- No inactive cell is allowed due to dry conditions when running the MT3D model

- No wells allowed in model layer 6

Formulation 2

Same as formulation 1, but assume diversion of 2400 gpm of extracted water (i.e., do not incur treatment cost or discharge cost for up to 2400 gpm of extracted water). Changes to the objective function are in the following terms:

CCT: Capital cost of treatment ($1,000/gpm)
CCD: Capital cost of discharge ($1,500/gpm)
VCT: Variable cost of treatment ($283/gpm/yr)
VCD: Variable cost of discharge ($66/gpm/yr)

In each case, cost must be calculated by subtracting 2400 gpm from the total pumping rate at remediation wells.

Formulation 3

The objective function is to minimize the maximum total remediation pumping rate in any management period over a 30-year simulation. The constraints are the same as for Formulation 1, except:

- The constraint requiring cleanup within 30 years is eliminated

- A constraint limiting the number of new remediation wells to 25 is added

In essence, this formulation is intended to determine the minimum pumping rate at any point in time that meets all remaining constraints (after the cleanup constraint is removed), including the constraint representing plume containment.

5. Performance Assessment

5.1 Performance Data

To assess performance of the transport optimization algorithms, the formulations described in Section 4 were solved by the UA team (using MGO), USU team (using SOMO3), and GeoTrans team (using trial-and-error search). Since both the MGO and SOMO3 packages contain multiple solution algorithms, different algorithms were used for different individual formulations based on modelers' expertise, as summarized below. The results from each of these two groups were compared to each other, and to the results of trial-and-error optimization performed by GeoTrans.

Please note that optimization results are not compared to the current system. The reason is that the current system was not designed with the current version of the groundwater model, nor was the current system designed to be optimal for any of the formulations solved in this study. Therefore, it is not fair to compare the current system to the optimal results, and there are no scientific conclusions that can be gained from such a comparison. The performance objectives associated with this study involve comparing objective function values of solutions obtained with transport optimization to objective function values obtained with trial-and-error. Reports from the individual modeling groups (included in the Appendices) at times compare solutions to the current systems as an intermediate benchmark, because the individual modeling groups did not have the results from the other modeling groups to compare their results to. However, this project summary report focuses on the comparison that is central to the project, which is the comparison of solutions obtained with transport optimization algorithms versus trial and error.

This project did not include detailed technical comparison of the numerical techniques implemented in the UA and USU codes, and rather focused on the results produced by each group. However, the method-specific parameters used by the UA and USU teams have been provided in the individual modeling report (Appendices D – F). Appendices D – F may be consulted for detailed reports on the approaches each team took at each site. Note that the comparison results tables provided in this section are intended to compare the broad optimization results (maximum or minimum objective function values and associated pumping strategy parameters) for the entire simulation period, and details such as the time variability of the pumping solutions obtained (i.e., pumping rate changes from one 3-5 yr management period to another) are included in the detailed reports.

5.1.1. Umatilla Performance Data

Overview of Solution Approaches

Both UA and USU started with Formulation 3, which they reported was the easiest of the three formulations to solve. Formulation 3 was simpler because it could be solved

sequentially in time without any loss of accuracy. That is, the first management period could be solved alone, minimizing mass remaining at the end of the first period. That mass remaining then became an initial condition for the second management period, which would then be solved to minimize mass remaining at the end of the second period. This process continues until the fourth management period solution is found. This approach allows the solution to the entire problem to be found sequentially with substantially less computational effort than finding the optimal solution for all four management periods simultaneously. Once Formulation 3 was solved in this manner, they then applied the knowledge learned from solving Formulation 3 when solving Formulations 1 and 2. The trial-and-error group started with Formulation 1. All three groups used results from Formulation 1 as the initial solution for Formulation 2.

The algorithms used for each formulation from the UA and USU teams are listed in Table 5-1:

Table 5-1. Algorithms Used By Transport Optimization Groups, Umatilla

	UA	**USU**
Formulation 1	TS	GA, then coupled GA and ANN
Formulation 2	TS	GA, then coupled GA and ANN
Formulation 3	TS and GA	GA

Both UA and USU teams reported that they solved subsets of entire formulations sequentially, rather than solving the whole problem at once, due to computational efficiency. The sequential modeling approach was used to either determine well locations first and then solve for the pumping rates, or to optimize pumping strategy sequentially for one management period at a time.

Umatilla Formulation 1 Results

Table 5-2 shows the results for Formulation 1, and Figure 5-1 shows the cumulative cost over time of the “optimal” results from the three groups. The USU and UA teams, which used optimization algorithms, found very similar solutions. To overcome computational limits, both teams applied sequential approaches to optimization, using multiple runs and approaches to explore possible solutions without solving the entire problem simultaneously.

Table 5-2. Umatilla Formulation 1 Results

	Transport Optimization Algorithms		Trial-&-Error
	UA	USU	GeoTrans
Objective Function Value	$1.66M	$1.66M	$2.23M
# New Extraction Wells	2	2	2
# New Infiltration Basins	0	0	1
# Existing Extraction Wells	2	2	3
# Existing Infiltration Basins	2	2	3
Elapsed Years Until Cleanup For RDX	4	4	6
Elapsed Years Until Cleanup For TNT	4	4	6

The UA team obtained their results using tabu search. Recognizing that the fixed annual labor and sampling costs dominated the cost function, the UA team simplified the objective function to minimizing the maximum concentrations of TNT and RDX in model layer 1 as quickly as possible while satisfying all the constraints. This was accomplished by starting with a predetermined duration of 20 years and then sequentially reducing the cleanup duration until no feasible solution (i.e., that met the TNT and RDX cleanup levels) could be found.

Prior to performing the optimization simulations, the UA team pre-supposed that up to four potential new pumping wells and up to three potential new infiltration basins would be sufficient for developing an "optimal" solution. The "moving cells" option in MGO was used to evaluate multiple candidate locations for these potential new wells and infiltration basins. This was done by associating each well or infiltration basin with a rectangular region of the model grid within which the well or infiltration basin can move freely in search of the optimal location.

In the USU approach, batches of candidate wells in groups were pre-defined, based on knowledge from solving Formulation 3. From these batches, the optimization model would select 2 new wells at a time – functioning like a "moving well approach" using sparse candidate well locations. The GA identified good well locations and pumping rates, which yielded the least-cost solutions. USU then obtained a slightly improved solution using a neural network trained to predict the effects of pumping rates at each well location on the constrained TNT and RDX concentrations. The optimal solution was verified to be feasible using the actual simulation model.

The GeoTrans team, which served as a control group by using a trial-&-error approach, found good solutions but were not able to match the solutions obtained by the teams applying the optimization algorithms. The trial-&-error solution was sub-optimal by

approximately 34%, based on objective function value, relative to the optimal solution determined with an optimization algorithm.

All three groups reported that their primary approach involved minimizing the cleanup time. For this specific formulation, the costs in the objective function are only incurred until cleanup is reached for both RDX and TNT, and the two dominant cost components, i.e., the fixed annual O&M labor cost and the variable sampling cost, depend directly on the number of years until cleanup. Therefore, rapid cleanup is desired. The UA and USU teams were able to improve their objective function values primarily by finding solutions with shorter total cleanup time (4 years) relative to the trial-&-error solution (6 years).

The optimal solution from all three groups used existing pumping wells EW-1 and EW-3, which are located in the TNT plume, plus two new wells also located within the TNT plume. TNT sorbs strongly to the soil and hence is more difficult to remove than the RDX. Therefore, having maximum pumping within the TNT plume is essential to ensure that the cleanup is completed as quickly as possible. All three optimal solutions used the two existing recharge basins located toward the south (IF2 and IF3) that were designed to flush the RDX towards the extraction wells.

The trial-&-error solution by GeoTrans also used existing well EW-4, which is in the center of the RDX plume, for the first five years. The UA and USU teams, operating with automated optimization techniques, learned that by shutting off well EW-4, more pumping could be applied within the TNT plume without exceeding treatment capacity. Under this approach, the RDX plume was effectively pulled toward the TNT plume due to the increased pumping in the TNT area. As a result, cleanup time for TNT could be shortened to 4 years while maintaining RDX cleanup within 4 years. The trial-&-error team never considered solutions with all pumping concentrated within the TNT plume. Therefore, they could not achieve cleanup within the TNT plume in less than 6 years because treatment plant capacity plus the pumping at EW-4 in the RDX plume limited the amount of potential pumping within the TNT plume. However, they did discontinue use of EW-4 after the first 5 years once RDX was largely remediated, re-allocating that pumping to other wells within the TNT plume for the sixth year.

The solutions by the UA and USU teams, operating with automated optimization techniques, avoid using the existing recharge basin north of the TNT plume (IF1) because it would hamper the ability of wells extracting water within the TNT plume to draw back the RDX plume to “clean” within 4 years. These groups shifted that infiltration to the basins south of the RDX plume, which in fact helps push the RDX towards the extraction wells. The trial-&-error solution by GeoTrans continued use of the northern infiltration basin (IF1) to speed TNT cleanup (to compensate for less pumping within the TNT plume in their solution), and also added a new recharge basin south of the TNT plume after 5 years to further speed the cleanup of the TNT plume.

The fact that all three groups added two new pumping wells within the TNT plume at various locations near EW-1 and EW-3 indicates the importance of maximizing pumping within the TNT plume to speed up TNT cleanup, based on model predictions. The

strategy of moving all pumping within the TNT plume is successful according to the model because of high hydraulic conductivity zones in layer 1 of the model (see Figure 5-2), which allow the RDX plume to be pulled to wells located in the TNT plume within just a few years. These modeled hydraulic conductivities are quite high and may be subject to uncertainty.

The USU team used their optimization model to identify hundreds of different paired locations (cells) for the two new wells in the TNT plume that could yield virtually the same objective function value. Pumping rates for the two new wells differed slightly. To help them select which well locations to recommend from among these hundreds, USU evaluated the locations based on robustness. Here, robustness is the likelihood that the RDX and TNT plumes would actually be cleaned up within four years in the field, even if field hydraulic conductivities differed from those assumed in the model. USU found and recommended that one of the two wells should be near the southern end of the TNT plume to increase RDX plume robustness. All three groups found that at least one new well needed to be north of the TNT hot spot.

The USU team also performed a limited post-optimization sensitivity analysis that showed that their optimal designs would be robust for variations in hydraulic conductivity of approximately10-15%. Greater variations might lead the strategy to fail, but whether the failure would lead to loss of capture or simply a longer remediation period is not clear without further analysis.

Umatilla Formulation 2 Results

Results for Formulation 2, in which additional GAC units could be added to the current treatment plant, are shown in Table 5-3.

Table 5-3. Umatilla Formulation 2 Results

	Transport Optimization Algorithms		**Trial-&-Error**
	UA	USU	GeoTrans
Objective Function Value	$1.66M	$1.66M	$2.02M
# New Extraction Wells	2	2	2
# New Infiltration Basins	0	0	0
# New GAC Units Installed	0	0	2
# Existing Extraction Wells	2	2	3
# Existing Infiltration Basins	2	2	3
Elapsed Years Until Cleanup For RDX	4	4	4
Elapsed Years Until Cleanup For TNT	4	4	4

The major difference in cost between the groups using transport optimization algorithms and the group using trial-&-error is that the trial-&-error solution required additional treatment capacity, with a capital cost of $300K, to achieve cleanup in 4 years (versus the trial-and-error solution of 6 years for Formulation 1). The groups using transport optimization algorithms achieved the 4 year cleanup time without additional capacity (i.e., using the solution to Formulation 1). The transport optimization modeling groups discovered that increasing pumping rate and adding a new GAC unit would not reduce the cost below the optimal solution to Formulation 1, thus they concluded that the optimal solution for Formulation 1 is also the optimal solution for Formulation 2. The trial-&-error solution was sub-optimal by approximately 22%, based on objective function value, relative to the optimal solution determined with an optimization algorithm.

Umatilla Formulation 3 Results

The objective for Formulation 3 is to minimize mass remaining (RDX plus TNT) in model layer 1 after 20 years. Table 5-4 compares the optimal solutions for Formulation 3, and Figures 5-3 and 5-4 illustrates the mass remaining of the optimal solutions for RDX and TNT, respectively.

Table 5-4. Umatilla Formulation 3 Results

	Transport Optimization Algorithms		**Trial-&-Error**
	UA	USU	GeoTrans
Objective Function Value	0.19 kg	0.20 kg	0.38 kg
# New Extraction Wells	2	2	2
# New Infiltration Basins	1	0	0
# Existing Extraction Wells	4	3	3
# Existing Infiltration Basins	2	2	3
Elapsed Years Until Cleanup For RDX	5	5	7
Elapsed Years Until Cleanup For TNT	3	4	7

As with the other formulations, the optimal solutions developed by the UA and USU teams, using optimization algorithms, are nearly identical, despite different solution approaches. The UA team used both tabu search and genetic algorithms for this formulation. Tabu search was initially used to identify well locations, assuming fixed pumping rates. Once the well locations were identified, both genetic algorithms and tabu

search were used to search for optimal pumping rates. The two algorithms were employed separately in parallel modeling efforts by the two investigators. In the search for optimal pumping strategies, optimization was performed for each management period sequentially. For example, one optimization run was done for Management Period 1 to minimize mass remaining. The mass remaining at the end of the first management period then became the initial conditions for minimizing mass remaining at the end of the second management period, and so forth.

The USU team began by allowing up to 2 new well locations in the first management period, with subsequent sequential optimization (i.e., potential for other new well locations) in subsequent management periods. After several runs USU concluded that adding extraction wells in the later management periods, besides the two new extraction wells installed in the first management period, would not be cost effective (though not rigorously accounted for in the formulation). Thus, later simulations were performed with the condition that installation of two new extraction wells would only occur in the first management period, with no new wells installed in subsequent management periods. The sequential GA optimization was then used to decide the locations for one or both of the wells and their rates.

The trial-&-error solution was sub-optimal by approximately 50%, based on objective function value, relative to the optimal solutions determined with the optimization algorithms.

Although cost is not considered in this formulation, and all three groups were free to add up to four new wells and three new infiltration basins, the optimal solutions provided by each group contained at most 2 new wells (again, located within the TNT plume), and only one group added a new infiltration basin. This appears to be a result of each group deciding that additional new wells and/or infiltration basins were not likely to be considered reasonable to the Installation, given the extremely low mass remaining that each group obtained, and therefore each group solved a more tightly constrained problem than they were actually allowed to solve (i.e., better objective function values might be mathematically possible if new wells or infiltration basins are added).

The GeoTrans solution obtained using trial-&-error used all three existing recharge basins, but the USU and UA solutions obtained with optimization algorithms used only the two southern recharge basins. The UA group also added a new recharge basin at the southern end of the RDX plume, which may have led to their slightly improved solution.

At first glance, this formulation appears to be less useful than the others, because the optimization results of Formulations 1 and 2 indicated the potential for cleanup in 4-6 years, while this formulation assumes pumping for a full 20 years. Also, because the concentrations and mass remaining in the latter years are so low, the model predictions are most likely to be in error because of the equilibrium adsorption assumed in the model. However, both groups applying optimization algorithms solved this formulation first, because it was the easiest to implement within the optimization algorithms. In the process of solving this formulation, they each learned that a solution existed that could

reach the cleanup levels within four years. These groups were then able to solve Formulations 1 and 2 with only one 5-year management period, which significantly reduced computational effort.

5.1.2. Tooele Performance Data

Overview of Solution Approaches

All three groups started with Formulation 1, then solved Formulation 2 based on the results from Formulation 1. Also, all three groups quickly concluded that no feasible solution could be found for Formulation 3 due to the constraint on the number of new wells allowed. Thus, various alternative formulations to Formulation 3 were developed and solved by each group.

The algorithms used for each formulation from the UA and USU teams are listed in Table 5-5:

Table 5-5. Algorithms Used By Transport Optimization Groups, Tooele

	UA	USU
Formulation 1	GA	GA
Formulation 2	GA and TS	GA
Formulation 3	GA	GA

As was the case for Umatilla, both UA and USU teams used sequential approaches instead of solving the whole problem simultaneously due to computational efficiency. The sequential modeling approach was used to determine the well locations first and then solve the pumping rates sequentially for each management period.

Tooele Formulation 1 Results

Table 5-6 shows the results obtained by each modeling group for Formulation 1. Figure 5-5 compares the cumulative cost over time of the results obtained by three groups.

Table 5-6. Tooele Formulation 1 Results

	Transport Optimization Algorithms		Trial-&-Error
	UA	USU	GeoTrans
Objective Function Value	$12.67M	$14.14M	$14.63M
# New Extraction Wells	0	3	4
# New Injection Wells	4	0	0
# Existing Extraction Wells Used	2	2	2
# Existing Injection Wells Used	1	11	8

All of the groups recognized that cost would be minimized at this site by minimizing the number of wells installed and operating, rather than by minimizing the cleanup duration as at the Umatilla site.

All of the teams found solutions that use only 2 of the 16 existing extraction wells, indicating that many of the existing extraction wells may not be needed to meet the facility's current objectives. The groups using mathematical optimization, UA and USU, found solutions that cost 13% and 3% less, respectively, than the trial-&-error solution from GeoTrans. Approximately $10M of the costs were fixed O&M costs and could not change with the pumping strategy, however. If these costs were removed, the mathematical optimization solutions were 42% and 11% less expensive than the trial-&-error solutions.

The USU and GeoTrans solutions used many of the existing injection wells combined with a few new extraction wells and no new injection wells, but USU found a solution that reduced the number of extraction wells installed from four to three by using more existing injection wells. The UA solution reduced costs (relative to both of the other groups) by using only new injection wells near the POE-MP constraint boundary (POE-MP shown in Figure 3-5). According to the cost function provided by the installation, extraction wells cost $84,000 more than injection wells to install, and extraction wells cost $34,500 per year to operate whereas injection wells have no annual operating costs. This makes injection wells more attractive cost-wise than extraction wells in the objective function.

The UA team pre-determined that four new extraction wells within a candidate region near the POE boundary would be sufficient to determine an "optimal" solution. The "moving cells" option in MGO was used to evaluate multiple candidate locations for the new wells within this region. They started with seeking steady-state solutions, i.e., the well locations and flow rates were assumed to be constant throughout all management periods. UA subsequently identified that feasible solutions could also be achieved with much lower cost by replacing the new extraction wells with injection wells. After the well locations were determined based on this steady-state approach, a final optimization

run was carried out to develop an optimal dynamic pumping strategy by treating flow rates for each management periods at each pumping/injection well as a decision variable.

The USU team did not allow injection wells within the plume in the POE area because of their concerns that injection without pumping could spread the leading edge of the plume. They solved the problem by first finding “optimal” solutions for the first management period only, and then after identifying a desirable batch of candidate well locations, they performed sequential optimization for the remaining management periods.

Tooele Formulation 2 Results

Table 5-7 shows the results obtained for Formulation 2.

Table 5-7. Tooele Formulation 2 Results

	Transport Optimization Algorithms		**Trial-&-Error**
	UA	USU*	GeoTrans
Objective Function Value	$14.45M		$16.32M
# New Extraction Wells	1		5
# New Injection Wells	7		3
# Existing Extraction Wells Used	2		2
# Existing Injection Wells Used	2		7

**The USU team did not submit a design for Formulation 2 as posed because they added a constraint to prevent potential for mass migration around the west side of POC-MP1, so their results cannot be compared directly to the other groups*

All of the groups found that injection just upgradient of the POC boundaries was the only way to meet the POC constraints as formulated. It is not clear that these solutions meet the intended benefit of the POC, which is to implicitly meet the POE-MP by achieving the POC constraints, because all of the solutions still require continued pumping at the POE-MP for the entire 21 year period.

The UA solution was 11% less expensive than the trial-&-error solution, which becomes a 30% improvement if the fixed O&M costs that cannot be changed with pumping are removed. The USU team did not submit a design for Formulation 2 *as posed* because they added a constraint to prevent potential for mass migration around the west side of POC-MP1 (POC-MP1 shown in Figure 3-5). The optimal solution for the problem as posed can cause mass loss around the POC to the northeast area, augmenting current mass losses in that area, and also to the west side of POC-MP1. USU added an additional constraint to prevent mass migration around the west side of POC-MP1, so their results cannot be compared directly to the other groups. With the additional constraint, the USU team found a solution that cost $17.1M during the modeling period and $15.73M about

two weeks later, before knowing the other team's solutions and as permitted by their contract.

The UA team solved the problem by obtaining the solution satisfying POC constraints regardless of the POE-MP constraint first, then adding the POE-MP constraint. The first attempt by the UA team determined that injection alone could satisfy the POC constraints under steady-state condition. Then the "moving cell" option was used to define a much larger candidate well region for injection wells. After the solution satisfying POC constraints was obtained, an optimal steady-state strategy was developed by adding the solution of Formulation 1 for the POE-MP, and optimizing from that point. To satisfy the balance of pumping and injection, one new pumping well and 3 new injection wells were used to satisfy POE-MP constraint instead of 4 new injection wells in Formulation 1. After the well locations were all fixed, the final optimal solution was obtained by optimizing the pumping/injection rates for each management period.

GeoTrans, the trial-and-error team, solved the problem by obtaining the solution satisfying POC-MP1 as well as POE-MP first, then adding the POC-MP2 constraint.

Tooele Formulation 3 Results

All three teams reported that Formulation 3 was infeasible as stated, due to the restriction on the number of new wells that could be installed. To eliminate this infeasibility, all of the groups chose to allow more new wells. Also, each group solved a slightly different problem (see Table 5-8) by modifying one or more constraints, so the results from each group are not directly comparable. Table 5-9 shows the results obtained for the alternative version of Formulation 3 solved by each group.

Table 5-8. Alternative Versions of Formulation 3 Solved by Each Group, Tooele

	Objective Function	Modified/Added Constraints
UA-1	Smallest # of new well required to satisfy all constraints	• Relaxed limit on number of new wells installed • Assume existing well screens can be modified to extract from a higher level
UA-2	Least total cost	• Relaxed limit on number of new wells installed
USU*	Least total cost	• Relaxed limit on number of new wells installed • Injection not allowed inside the plume except a specified area • Containment constraint at the west edge of the plume in first 9 years to reduce mass migration
GeoTrans	Least total cost	• Relaxed limit on number of new wells installed

**USU completed this problem about 2 weeks after the 4-month modeling period*

Table 5-9. Tooele Alternative Formulation 3 Results

	Transport Optimization Algorithms			**Trial-&-Error**
	UA – 1	UA – 2	USU	GeoTrans
Objective Function Value	$19.3M	$18.6M	$17.9M	$18.6M
# New Extraction Wells	4	5	9	9
# New Injection Wells	6	7	3	4
# Existing Extraction Wells Used	6	3	3	2
# Existing Injection Wells Used	0	0	0	0

**Note: Each Group Solved a Different Formulation, Results Not Directly Comparable*

The UA team examined two different alternative formulations using genetic algorithms. The first alternative was to identify the smallest number of new wells that would be required to obtain a feasible solution. They found a solution that used 4 new extraction wells, 6 new injection wells, and 6 existing wells, at a cost of $19.3M. The second alternative was to identify the least cost solution that would allow the number of new injection wells and new pumping wells to exceed the original constraint, which had a solution with 5 new extraction wells, 7 new injection wells, 3 existing wells, and a cost of $18.6M. Their solutions all employed steady pumping rates over time, but some wells were pumping clean water by the end of the modeling period and could be candidates for shutting down and saving additional costs with further optimization. Their solutions also allowed pumping in existing wells at higher screen intervals relative to existing well screens, assuming that existing well screens could be modified at no cost to allow this solution.

The USU team used genetic algorithms to identify a solution with 9 new extraction wells, 3 new injection wells, 3 existing extraction wells, and a cost of $17.9M. This solution was found shortly after the modeling period ended, as was permitted when the formulation was infeasible. In identifying this solution, the USU team did not allow injection at locations within the plume other than near POC-MP1. As with Formulation 2, they also included an additional constraint limiting concentrations around the western edge of POC-MP1, but did not apply that constraint in the last period to reduce costs.

Finally, the trial-&-error team found a solution with 9 new extraction wells, 4 new injection wells, 2 existing extraction wells, and a cost of $18.6M. This solution was obtained by relaxing the constraint on the number of new wells and satisfying all other original constraints. They also performed a series of three additional simulations to try to improve other objectives (improving cleanup between the bedrock block and POE, removing more mass, and preventing loss of mass to the northeast). While some improvements were noted, costs increased substantially (see Appendix E for more details) and the group did not recommend that these alternate solutions be considered for implementation.

Although each of the three groups solved slightly different problems, the objective function values found were similar. The optimal well locations and strategies were also highly constrained by locations of continuing sources. In fact, many extraction well locations that were selected are near continuing sources.

It should be noted that some locations of fractured bedrock in the main plume were exempted from the cleanup constraints in the formulation, because it was felt that cleanup could not be achieved at those locations in the model because of the low hydraulic conductivity. Also, several locations where source strength exceeds 50 ppb at the end of year 9 in model layer 1 and their surrounding locations are exempted from the cleanup constraints because the model will not predict concentrations below 50 ppb at those locations. Hence, significant contaminant mass and the contaminant plume are still present even when this "cleanup constraint" is satisfied.

5.1.3. Blaine Performance Data

Overview of Solution Approaches

Both the UA and USU groups solved Formulation 1 first, then Formulation 2 and then solved Formulation 3. The trial-and-error team started with Formulation 3 (after a few initial simulations for Formulation 1) because it was the easiest problem to find a feasible solution for (no cleanup constraint), then solved Formulation 1 based on knowledge learned from solving Formulation 3, and finally achieved optimal solution for Formulation 3 based on optimal solution for Formulation 1. The trial-&-error group never performed any actual simulations for Formulation 2. Instead, they used a logical premise for concluding that the optimal solution for Formulation 1 would also be optimal for Formulation 2.

The algorithms used for each formulation from the UA and USU teams are listed in Table 5-10:

Table 5-10. Algorithms Used By Transport Optimization Groups, Blaine

	UA	USU
Formulation 1	TS and GA	GA, SA, GA coupled with ANN
Formulation 2	TS and GA	GA, SA, GA coupled with ANN
Formulation 3	TS and GA	GA

Due to the long computational time, about 2 hours per simulation, both groups using optimization algorithms used a sequential approach. The UA team solved each formulation sequentially in time, starting in period 1, then periods 2, 3, 4, 5, and finally

period 6. They also determined optimal well locations first, then solved the time-varying pumping rates. Similarly, the USU team developed time-varying pumping strategies after first determining optimal well locations with GA. However, the USU group then solved for all management periods at one time (not one management period at a time) using GA, SA, and GA coupled with ANN, which in some cases were used for compare algorithms.

Blaine Formulation 1 Results

Table 5-11 shows each team's results for Blaine under Formulation 1. Figure 5-6 compares the cumulative cost over time of the results obtained by three groups.

Table 5-11. Blaine Formulation 1 Results

	Transport Optimization Algorithms		**Trial-&-Error**
	UA	USU	GeoTrans
Objective Function Value	\$45.28M	\$40.82M	\$50.34M
# New Extraction Wells	15	10	8
Pumping Rates By Management Periods	1968 gpm 3104 gpm 3356 gpm 3700 gpm 3750 gpm 3750 gpm	2486 gpm 2632 gpm 2644 gpm 2752 gpm 3306 gpm 3378 gpm	3995 gpm 3975 gpm 3995 gpm 3995 gpm 3925 gpm 3105 gpm
Elapsed Years Until Cleanup for TCE	30	30	30
Elapsed Years Until Cleanup for TNT	30	29	25

For this site and formulation, all three groups found that the least cost solutions came from minimizing pumping in each management period, not shortening the cleanup duration. All of the groups' solutions for model layer 3 involved installing at least one well in the toe of the TNT plume, and at least one well northwest of the main TCE plume where high levels of TCE leak from model layer 2 (Figure 5-7).

Both groups using optimization algorithms found better solutions than the trial-&-error group. The USU team's solution was approximately 20% improved over the control group and the UA team's solution was approximately 10% improved over the control group. Both groups employed an approach with more wells and increasing pumping rates at later management periods, while the trial-and-error group installed wells at early periods and then lowered the pumping rates at later management periods (see Table 5-11). The UA group employed sequential solution approaches (described earlier) to overcome computational limits, which were particularly acute at this site (each simulation run took about 2 hours on a Pentium III 1-GHz PC).

The USU team used genetic algorithms to identify well locations based on pre-determined candidate well locations, keeping the managed wells under steady pumping for 30 years. The USU team then used GA, SA, and GA plus ANN to develop steady and/or transient 30-year pumping strategies for the sets of candidate wells identified previously.

The UA team used both genetic algorithms and tabu search in parallel runs to determine the well locations. The initial locations of remediation wells were pre-determined manually. The final locations were optimized through tabu search and genetic algorithms by defining a candidate region for potential well locations. After the well locations were determined, the pumping rates were fine-tuned by applying a surrogate model approach that was similar to USU's approach. However, they fit a quadratic response function to the pumping rates at each well location instead of ANN. They also solved the problem sequentially in time, finding an optimal solution for each management period separately, without considering subsequent management periods.

Blaine Formulation 2 Results

Table 5-12 shows the results for Formulation 2. All three groups found that the solution that was optimal for Formulation 1 was also optimal for Formulation 2. Diverting part of the extracted water reduced treatment costs substantially, but did not change the optimal pumping strategy.

Table 5-12. Blaine Formulation 2 Results

	Transport Optimization Algorithms		**Trial-&-Error**
	UA	USU	GeoTrans
Objective Function Value	$24.04M	$18.88M	$28.39M
# New Extraction Wells	15	10	8
Elapsed Years Until Cleanup for TCE	30	30	30
Elapsed Years Until Cleanup for TNT	30	29	25

With the reduced treatment costs, the optimal strategy from the USU and UA teams were about 33% and 15% less expensive, respectively, than the trial-&-error team's solution. The UA team's solution would allow all of the water extracted during the first management period to be diverted, potentially eliminating the need to install a treatment plant for 5 years. This would only be possible if the TNT levels in the water were low enough to allow diversion of all the water, however. Neither the USU solution nor the trial-&-error solutions pump less than 2400 gpm in the first management periods, so those solutions both require a treatment plant at the beginning of the remediation.

Blaine Formulation 3 Results

Table 5-13 shows the results for Formulation 3.

Table 5-13. Blaine Formulation 3 Results

	Transport Optimization Algorithms		**Trial-&-Error**
	UA	USU	GeoTrans
Objective Function Value	2737 gpm	2139 gpm	2879 gpm
# New Extraction Wells	13	25	7
Pumping Rates By Management Periods	2730 gpm 2737 gpm 2737 gpm 2732 gpm 2592 gpm 2397 gpm	2139 gpm 2139 gpm 2139 gpm 2139 gpm 2139 gpm 2129 gpm	2879 gpm 2879 gpm 2879 gpm 2879 gpm 2879 gpm 2879 gpm
Elapsed Years Until Cleanup for TCE	>30	>30	>30
Elapsed Years Until Cleanup for TNT	30	>30	30

Again, both groups using optimization algorithms achieved better solutions than the trial-&-error group, with the USU team's solution having 26% improvement and the UA team's solution having 5% improvement. All three groups obtained significantly different solutions, with peak pumping rates ranging from 2,137 to 2,879 gpm and 7 to 25 pumping wells (note that the number of wells, cost, and the cleanup time were not optimization criteria for this formulation). Solutions that used more wells had lower peak pumping rates, as would be expected.

The UA team solved the problem using the same approach as for Formulation 1, determining the well locations using tabu search and genetic algorithms, then obtaining the pumping rates by applying a surrogate model, i.e., a response function.

The USU team solved the problem by assuming steady pumping for managed wells and using genetic algorithms and simulated annealing at first, then optimized time-varying pumping using genetic algorithms coupled with artificial neural network, as with Formulation 1.

Although this containment formulation did not require cleanup, all three optimal solutions came close to satisfying the cleanup constraints from the previous formulations. However, the objective of minimizing pumping did allow some plume growth within the containment zone. The USU team examined alternate formulations that allowed less plume growth (see Appendix F). Finally, it should be noted that the USU solution may

not require treatment plant installation if the 2,400 gpm diversion proposed in Formulation 2 occurred and TNT levels in the water were sufficiently low.

5.2 Data Assessment

For all three sites, there were two groups applying optimization algorithms, and one group applying trial-&-error as a scientific control. For each of the three sites, multiple formulations were solved by each group. In each and every case, the groups applying the optimization algorithms found improved solutions relative to the trial-&-error group. Because multiple sites were evaluated, and multiple formulations for each site were evaluated, there is a high degree of confidence in the conclusion that the application of optimization algorithms provides improved solutions for problems posed in the manner demonstrated in this project (i.e., mathematical formulations with an objective function to be minimized/maximized and a series of constraints).

Both teams applying mathematical optimization obtained similar results for Umatilla, but the pumping strategy results differed considerably for Tooele and Hastings. The differences may be due to one or several of the following factors:

(1) Changes that individual modelers made in the formulations (primarily additional constraints) to overcome perceived problems in the solutions they obtained;

(2) Different approaches taken to overcoming the computational barriers of solving these complex problems;

(3) Convergence of the heuristic optimization algorithms to sub-optimal solutions;

The first factor arose because of the structure of this demonstration, in which each team worked in isolation for four months without presenting any initial results to the installation (to ensure independence of each team's results). When this technology has been applied at other sites by a single optimization team, initial results are presented to the installation and the formulations (i.e., objective functions and constraints) are modified as needed to overcome any difficulties identified in the initial solutions. Hence, this factor will not be an issue in future use of this technology. The second factor will likely remain in the foreseeable future. The last factor is intrinsic to the heuristic algorithms used in this optimization effort. If the optimization parameters were set appropriately, however, convergence to sub-optimal solutions should occur rarely. Hence, we expect that most of the differences in the mathematical optimization groups' results are due to the first two factors.

Two other considerations should be noted in assessing the results of this project. First, the optimization problems and the resulting solutions are defined by the objective function and the constraints. In this demonstration project, the formulations (including the detailed coefficients associated with the objective function and constraint terms) were developed in consultation with site installations or site managers. Relative to objective functions

previously used by other studies, the problems solved in this demonstration project are relatively complex and incorporate significant realistic detail. Relative to all of the real-world complexity that exists at these sites, the objective function and constraint terms by necessity include some simplifications. Obviously, changes to the objective functions and/or constraints, such as extending cleanup constraints for a longer duration of time, incorporating additional mathematical constraints, or removing constraints, could result in different solutions.

A second consideration in assessing these results is that with difficult nonlinear optimization problems such as the nine formulations solved in this project, there is no way to prove that the absolute global optimum has been found because the algorithms are heuristics and the solution space is astronomically large for a typical nonlinear optimization problem. The global optimization methods are “intelligent” search algorithms that attempt to get to a near-global optimum by only searching a small fraction of the entire solution space. To check if the global optimum is achieved, ideally one would run the optimization algorithm several times with different starting points to see if the results differ, and/or modify other input parameters associated with the specific algorithm, and/or attempt to solve the problem with other algorithms. However, that is not always possible for very computationally intensive problems like the sites demonstrated in this study. Nevertheless, the algorithms used in this study have been shown in practice to produce optimal or near-optimal solutions to a broad range of problems in other fields. More importantly, as indicated in Table 5-14 below, the global optimization methods clearly search a much larger portion of the solution space than the trial-&-error method and produce better solutions than trial and error. Given the computational limits, it is not practical to search the entire solution space so there is always a chance that global optimal solution will be missed, but for the problems solved in this project better solutions were consistently found by the transport optimization algorithms than with trial-&-error.

It should also be noted that, in this project, the transport optimization teams were generally provided with an initial feasible solution by the trial and error group to use as a “launching point”, but it is considered likely that the teams would have independently determined such an initial solution if they had not been provided with one. Table 5-14 summarizes the approximate number of runs performed by transport optimization teams versus the trial-&-error team for each of the three sites. Generally “simulations” refers to the number of iterations through the groundwater model, however, due to the use of substituted functions in place of the numerical model in some formulations, it is impossible to calculate the number of completed groundwater model simulations performed for the optimization codes more exactly.

Table 5-14. Approximate Number of Simulations Performed For Each Formulation

	Transport Optimization Algorithms UA and USU Teams	**Trial-&-Error** GeoTrans
Umatilla	~ 1000 – 8000 simulations	~ 25 – 40 simulations
Tooele	~ up to 8000 simulations	~ 60 – 80 simulations
Blaine	~ Hundreds/thousands simulations	~ 60 simulations

The optimization period for each site (once the formulations were established) was approximately four months. Each group was required to solve three problems and submit the optimal solutions within the timeframe of four months. Based on the improved solutions obtained, this illustrates that developing optimal solutions using transport optimization algorithms within a several month period is reasonable for problems where each model simulation requires 2 hours or less and up to 2 constituents are simulated.

This project did not evaluate the impact of uncertainty in model parameter values on the results of the optimization solutions. However, this issue could be evaluated in future projects either by examining the impact to optimal solutions from varying model parameter values or by using stochastic optimization methods to identify optimal solutions that are robust despite the uncertainty.

5.3 Technology Comparison

The results presented in Section 5.1 clearly indicate that mathematical optimization methods are able to identify solutions that are better than those obtained using traditional trial-&-error approaches. The solutions found were 5% to 50% better than those obtained using trial-&-error (measured using optimal objective function values), with an average improvement of about 20%. For Blaine, which has substantial costs, these results could give cost savings of up to $10M over the 30-year duration considered in the optimization scenario. The cost savings at Umatilla for an optimized cleanup strategy would be lower, with savings perhaps up to $600,000, but the Umatilla cleanup is much less expensive and complex than the Blaine site.

However, the challenges in applying optimization algorithms also increased with the complexity of the site. The greatest challenge that the optimization modeling teams faced was the computational requirements of the optimization algorithms. If a single optimization run were set up to solve the entire problem as formulated, with all possible pumping rates and well locations in all potential management periods, the number of decision variables would be much larger and the computational times associated with the optimization algorithms would be prohibitive on today's computers. Instead, the teams employed sequential solution approaches to reduce computational effort, in which some

parts of the problem were fixed while others were optimized. These approaches require substantial expertise and professional insight.

A limitation of the trial-&-error approach is that the objectives and constraints are often not rigorously stated. Another limitation is that there are an infinite number of combinations for well locations and well rates that are possible, but the trial-&-error method is practically limited to only a small number of numerical simulations (typically 10 – 50). The transport optimization codes more efficiently evaluate the potential solution space, such that many more combinations of extraction and injection well rates and locations can be evaluated (as shown in Table 5-14). Also, transport optimization is less prone to bias in selecting well rates and well locations because it is more automated than trial-&-error, and therefore is more likely to discover unexpected solutions.

6. Cost Assessment

6.1 Cost Performance

Based on the competitive bids evaluated in this project for selecting the transport optimization groups, plus the costs associated with GeoTrans' participation in the project, the expected costs (and expected time duration) of applying this technology at a future site is approximated in Table 6-1. The estimated range in costs results from differing site and model complexities. The actual costs associated with this demonstration project will be documented in the associated Cost & Performance Report.

Table 6-1. Approximate Cost To Apply Transport Optimization Algorithms at a Site

	Low Cost	Typical Cost	High Cost	Expected Duration
A1) Site Visit and/or Transfer Information	$2,500	$5,000	$10,000	1-2 months
A2) Develop 3 Optimization Formulations	$5,000	$10,000	$15,000	1-2 months
A3) Solve Optimization Formulations	$25,000	$40,000	$60,000	2-4 months
A4) Prepare Report and/or Present Results	$5,000	$15,000	$25,000	1 month
A5) Project Management and/or Administration	$2,500	$5,000	$10,000	NA
Total	***$40,000***	***$75,000***	***$120,000***	***5-9 months***

* *assumes 1 or 2 constituents, and simulation time of 2 hours or less*

Table 6-1 (cont'). Optional Items

	Low Cost	Typical Cost	High Cost	Expected Duration
B1) Update and Improve Models	0	$20,000	$50,000	Add 1-3 months
B2) Up To 3 Additional Formulations	$15,000	$25,000	$40,000	Add 2-3 months
B3) Additional Contaminant	$10,000	$20,000	$30,000	Add 1-2 months
B4) Transport Simulation of 3 hrs each (i.e., 1 hr longer)	$10,000	$20,000	$30,000	Add 1-2 month

6.2 Cost Comparisons to Conventional and Other Technologies

The appropriate item to compare in this section is the cost associated with Item A3 in Table 6-1. The issue is the extent to which application of transport optimization algorithms cost more than the application of trial-&-error, coupled with the anticipated life-cycle cost-savings that might be afforded by the application of transport optimization algorithms versus use of trial-&-error.

As shown on Table 6-1, the estimated cost of applying transport optimization algorithm (Item A3) for problems like those formulated for this project is approximately $25,000 to $60,000 (i.e., up to 2 constituents, simulations up to 2 hrs long, up to 3 formulations). The cost for the trial-&-error group for Item A3 for this project was approximately $30,000 per site, although that group reported for each site that it would have performed fewer simulations if not done within the context of this demonstration project. Thus, it is assumed that for comparable projects (i.e., up to 2 constituents, simulations up to 2 hrs long, up to 3 formulations) trial-&-error may cost approximately $20,000 to $25,000. Therefore, the premium for applying the transport optimization may be as little as zero, or as much as $40,000.

The improvements in objective function values achieved in this demonstration project with transport optimization algorithms (versus trial-&-error methodology) is anywhere from 5% to 50%, with a typical value of 20% to 30%. Assuming the objective function is in terms of cost, the potential life-cycle cost savings associated with the application of transport optimization algorithms will almost certainly exceed the premium of up to $40,000 for applying the technology at most sites that satisfy the simple site-screening criteria (more than $100,000/years in annual O&M and expected duration of 5 years or more). Obviously, for sites with high costs and/or high durations, such as a yet-to-be constructed pump and treat system where fewer cost and design parameters are fixed, the potential life-cycle cost savings become more significant. For example, in the Blaine demonstration, potential cost savings of approximately $10 million were identified relative to the trial-&-error solutions.

For cases where the objective function is not in terms of life-cycle cost, the cost-benefit evaluation is less straightforward (e.g., almost 50% less mass remaining in layer 1 for Umatilla using optimization algorithms versus trial and error). It is hard to quantify the extent to which a reduction in mass remaining, or an increase in contaminant removed, correlates to additional cost associated with application of transport optimization. However, as discussed earlier, the premium of applying transport optimization algorithms (up to $40,000) instead of trial-and-error method is not so high that it would be prohibitive for most sites to consider the transport optimization approach, such that qualitatively it appears that use of transport optimization should be encouraged. Additional investment may be required for uncertainty analysis of the underlying simulation model on the optimal solutions, but such analyses would be performed for the trial-and-error method as well.

7. Regulatory Issues

7.1 Approach to Regulatory Compliance and Acceptance

There are no regulatory issues that needed to be directly addressed beyond those that constrain the design and operation of the pump and treat systems being examined. Those regulatory issues were represented by the installation and considered during the development of the mathematical formulations that were solved using the transport optimization algorithms. The ESTCP project team encouraged regulatory participation in the process and for each demonstration site offered to help site personnel communicate with their regulatory partners regarding the optimization technology. However, installation personnel were ultimately responsible for keeping regulators involved in the project to the extent they desired.

At each of the three demonstration sites, potential modifications to an existing pump and treat system were suggested by the results. These may include changes in pumping rates at existing wells, or additional locations for pumping and/or injection. The specific installations will determine whether or not results from the demonstration project merit actual changes to the existing system, which would require subsequent regulatory interaction. At the request of the installation, project team members are willing to present the site-specific findings of the demonstration project to regulators based on final results obtained. In fact, Oregon regulators attended the Umatilla briefing where the project team presented the final results. The ESTCP project team continues to offer assistance in that regard if requested.

Members of the project team (e.g., Kathy Yager from EPA-TIO and Dave Becker from USACE HTRW-CX) have opened a dialogue with the ITRC (Interstate Technology and Regulatory Council) to describe the scope of this project, the general results, and potential range of application for future projects. In addition, Ms. Yager arranged for a presentation to EPA-NARPM (National Association of Remedial Project Managers) in 2003, to increase awareness of regulators regarding the transport optimization technology and the results of this demonstration project.

In addition, the technology demonstrated in this project can potentially be applied or recommended by regulators and/or their contractors to evaluate remediation scenarios at sites they manage and/or regulate. Training will be required to educate the regulatory and environmental community as to what can be accomplished with an algorithmic approach to P&T optimization, as well as to emphasize the limitations of the optimization algorithms related to uncertainties in the underlying model simulations.

8. Technology Implementation

8.1 DoD Need

This demonstration project shows that the potential for tremendous cost savings exists with the application of simple screening tools and optimization-simulation modeling. This supports the following Navy EQ user requirements (Table 1-1): 1.I.1.e improved remediation of groundwater contaminated with non-halogenated hydrocarbons; 1.I.1.g improved remediation of groundwater contaminated with halogenated hydrocarbons and other organics; and 1.II.1.a improved fate, effects and transport models for groundwater.

It is expected that the application of transport optimization codes could benefit some significant percentage (perhaps as much as 25% - 30%) of the over two hundred DoD pump and treat sites currently in operation. While the total cost benefit will vary with the expected lifetime of the specific pump and treat system, substantial potential life-cycle cost savings at the three demonstrations were suggested. Moreover, the remediation effectiveness (e.g., shorter contaminant cleanup duration) may also be improved for some pump and treat sites.

Reducing the operating costs of long-term remedial systems, inclusive of pump and treat systems, is an ongoing need. As detailed in the cost benefits screening evaluation tool used to qualify pump and treat systems for this optimization effort, as well as in the optimization results presented in this report, the pump and treat systems with annual cost of $100,000 or higher and total pumping rate of 50 gpm or higher, will usually achieve cost benefit from pumping reduction and/or operation duration reduction with application of transport optimization approaches. Such application requires development of a reliable underlying groundwater flow and solute transport model.

8.2 Transition

This technology can be implemented at the present time, but the codes have not previously been publicly available so it has been necessary to contract directly with one of the code developers to apply the technology. This is being mitigated as part of the technology transfer aspects of this project. The vendors have been requested to submit a usable version of their implemented codes for accessibility from a federal website on the internet (to be live on the internet by September 2003 at http://www.frtr.gov/optimization/simulation/transport/general.html). Availability of transport optimization codes will enable more widespread application of the technology by others who have suitable training. A further transition step was expected to include the incorporation of one or more of these transport optimization codes into an existing graphical user interface (GUI) for groundwater modeling. However, the investment required was deemed not beneficial at the current stage of code development, and the education steps are considered a higher priority. Although industry has not been involved

with the ongoing project, industry clients are likely to be interested in the technology demonstrated herein.

Training will be another aspect of the remaining project tasks associated with technology transfer. Training materials pertaining to the process of developing optimization formulations were developed by June 2003, and presented at the ASCE Environmental & Water Resources Institute - World Water & Environmental Resources Congress 2003 (Philadelphia, PA; June 23 – 26, 2003). A 2.5-day training course regarding the actual use of the optimization codes is also planned March 2004 at the International Ground Water Modeling Center in Golden, Colorado. An outline for 1-day and 2-day training courses has already been developed (Appendix C). Additionally, the individual transport optimization modelers each perform independent training (for a fee) on their codes on an ongoing basis.

Materials for a 2-hour internet seminar regarding this project have been developed. This internet seminar is sponsored by EPA-TIO (www.clu-in.org). A dry run was conducted on August 20, 2003, and the first delivery is scheduled on September 24, 2003.
To increase awareness regarding the technology demonstrated in this project, several conference presentations have been made at federal agency conferences, and future presentations are planned. These are summarized below.

Already Conducted

- ESTCP/SERDP Conference - Partners in Environmental Technology Technical Symposium & Workshop (Washington, DC; December 3 – 5, 2002). Poster & Presentation

- 2003 Navy/Marine Corps Cleanup Conference (Port Hueneme, CA; February 11 – 13, 2003)

- AFCEE 2003 Technology Transfer Workshop (San Antonio, Texas; February 24 – 27, 2003)

- ASCE Environmental & Water Resources Institute - World Water & Environmental Resources Congress 2003 (Philadelphia, PA; June 23 – 26, 2003).

- Tri-Service Workshop with ITRC (Charlotte, NC; March 25 – 28, 2003)

- US Army Corps of Engineers Environment and Natural Resources Conference (Fort Worth, TX; April 28 – May 1, 2003)

Planned

- MODFLOW and More 2003: Understanding through Modeling Conference (Golden, Colorado; September 16 – 19, 2003).

- UMass/AEHS Conference - The Annual Conference on Contaminated Soils, Sediments, and Water (Amherst, MA; October 20 – 23, 2003).

- USEPA Optimization Conference (2004)

- Battelle Conference - Fourth International Conference on Remediation of Chlorinated and Recalcitrant Compounds (Monterey, CA; May 24 – 27, 2004).

8.3 Status of System Modifications

Currently, both the Umatilla and Blaine teams plan on using the results of the ESTCP demonstration project as a basis for future operational changes. The Umatilla project team has ceased use of one infiltration basin based on the recommendation of the optimization teams and are in the process of seeking funds to update the ground water flow and transport models to reflect new site characterization data before revisiting the optimization further. The Blaine project team is considering the optimization recommendations as they proceed with preparation of a Proposed Plan and Record of Decision. They, too, are planning to update their model based on recent minor site characterization efforts. Both site teams indicated they would strongly consider applying optimization algorithms in conjunction with the updated models. The Tooele project team has been directed to investigate a temporary (two-year) termination of the operation of the pump and treat system to evaluate various processes affecting contaminant fate. The implementation of any of the optimization recommendations will be postponed pending this evaluation. Overall, the installations were very open to the recommendations and are implementing the recommendations to the extent possible given other constraints.

9. Lessons Learned

The optimization algorithms allow many more simulations to be performed within a fixed time period. In this demonstration project, thousands of simulations for each problem were performed by groups using optimization algorithms versus dozens of trial-&-error runs. Additionally, the transport algorithms may attempt solutions that would not be considered by a trial-&-error modeler (due to a pre-conceived bias and/or small number of trial-&-error simulations possible). This was the case at Umatilla, where the trial-&-error group never considered pumping only in the TNT plume area. This was also the case at Tooele, where the UA group was able to identify an injection-only solution near the POE boundary that was not obvious to the trial-&-error group.

This project clearly demonstrated that mathematical optimization is capable of identifying substantially improved solutions to real-world problems encountered for optimization of pump and treat systems. The cost benefits from applying the technology with an existing groundwater flow and transport model are greater at more complex sites such as Blaine, but the percentage improvements at simpler sites such as Umatilla can still be substantial. At all three sites, the projected cost savings outweighed the expected costs of applying the technology.

The development of mathematical formulations of the optimization problems was a difficult and time-consuming process. However, this formulation process results in a concise and quantifiable statement of project objectives and constraints not only necessary for transport optimization algorithms but useful for trial-and-error method as well. In that respect, the formulation process is worthwhile whether or not mathematical optimization algorithms are ultimately applied.

Some modifications to the existing flow and transport model were necessary prior to the optimization. These modifications included changes to model time discretization to correspond with management periods in the optimization formulations, simulating the model under current conditions into the future to provide initial conditions for the optimization simulations, and modifying the model solution package parameters to shorten computational time because the model runtime is the limiting factor for transport optimization algorithms to investigate a greater number of potential solutions. Also, many test runs were performed prior to performing optimization simulation to ensure the existence of a feasible solution for the technology comparison. This final step would not normally be required for application of optimization algorithms to field sites in the future, since the algorithms can identify infeasibilities.

Due to the specific needs of this demonstration project, the optimization formulations were fixed at the beginning of the simulation period, and simulation period length was defined. However, normally the optimization modeler would interact with the installation to develop revised formulations as optimization proceeds, and to adjust to new

knowledge. This project demonstrates that such iterations should be a useful component of real-world applications.

This project also demonstrated that applying the transport optimization algorithms was more than just "hitting the go button". It required expertise to limit the potential solution space to be searched. If a single optimization run were set up to solve the entire problem as formulated, with all possible pumping rates and well locations in all potential management periods, the number of decision variables would be much larger and the computational times associated with the optimization algorithms would be prohibitive on today's computers. Instead, the transport optimization teams employed sequential solution approaches to reduce computational effort, in which some parts of the problem were fixed while others were optimized. In some cases, problems were solved one management period at a time, and/or determining well locations first assuming steady-state pumping rates followed by optimizing well rates for those pre-determined well locations. These approaches require expertise and professional insight.

Both optimization codes demonstrated, MGO and SOMO3, include multiple algorithms for minimizing or maximizing the objective function, and expertise/insight is required to select the appropriate algorithm. Surrogate function approaches, such as artificial neural networks and other response functions, were used successfully at Blaine for reducing model computational time, thus enabling more effective solutions to be found, but these approaches also require expertise and professional insight to implement.

Finally, this project did not evaluate the impact of the uncertainty of simulation model parameters on the optimization solutions. However, this issue could be evaluated in future projects either by examining the impact on optimal solutions of varying model parameters or by using stochastic optimization methods to identify optimal solutions that are robust despite the uncertainty. Uncertainties in the model predictions have an associated impact on determination of an optimal solution and the robustness of that solution, and may impact the willingness of site managers to invest in system upgrades based on modeling. However, those issues pertain equally to any design based on flow and transport modeling, whether obtained using transport optimization algorithms or trial-&-error techniques.

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FIGURES

Figure 1-1. Site Location Map for Three Selected Sites

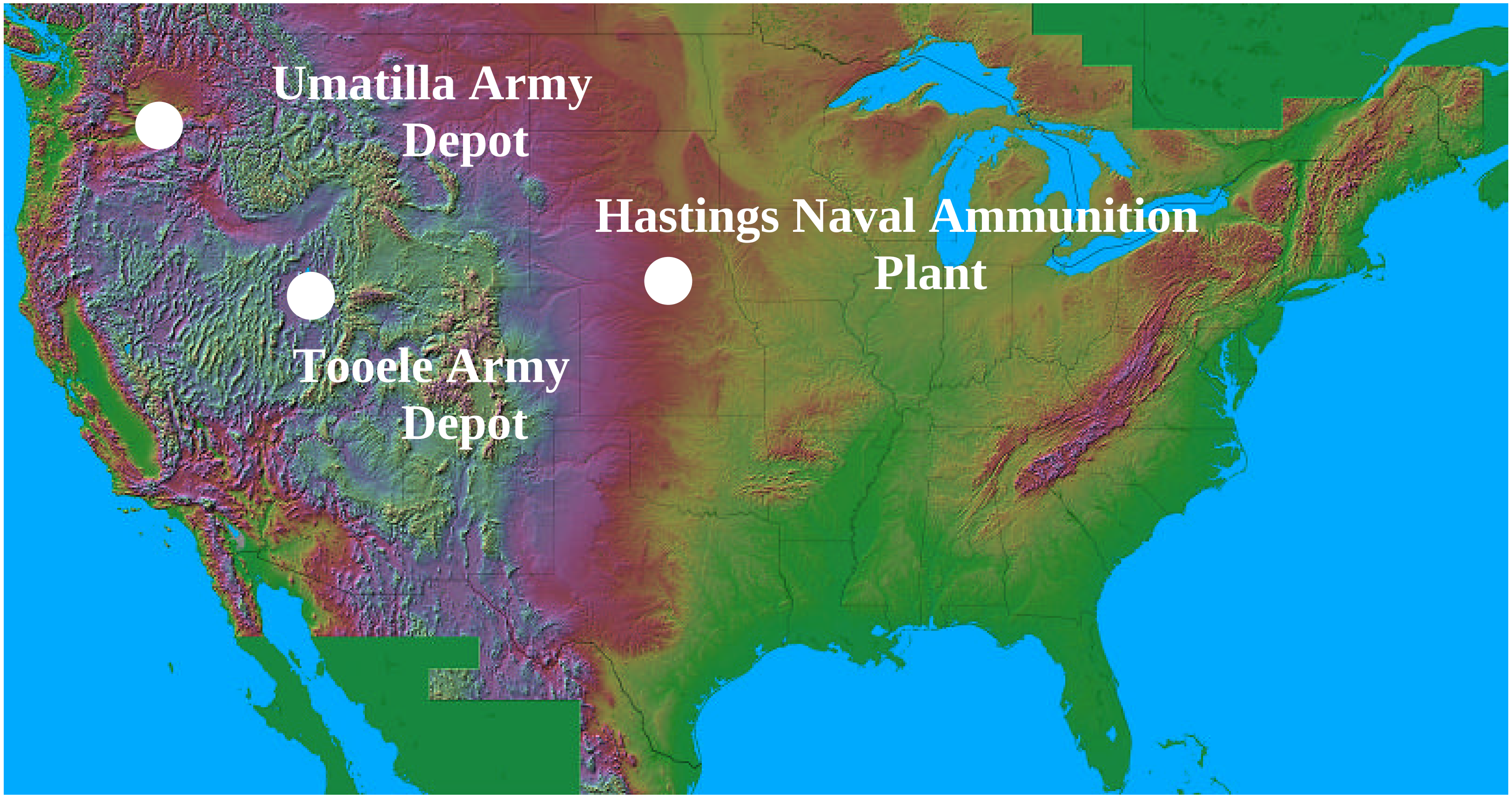


Figure 3-1. Site Location Map, Umatilla Chemical Depot

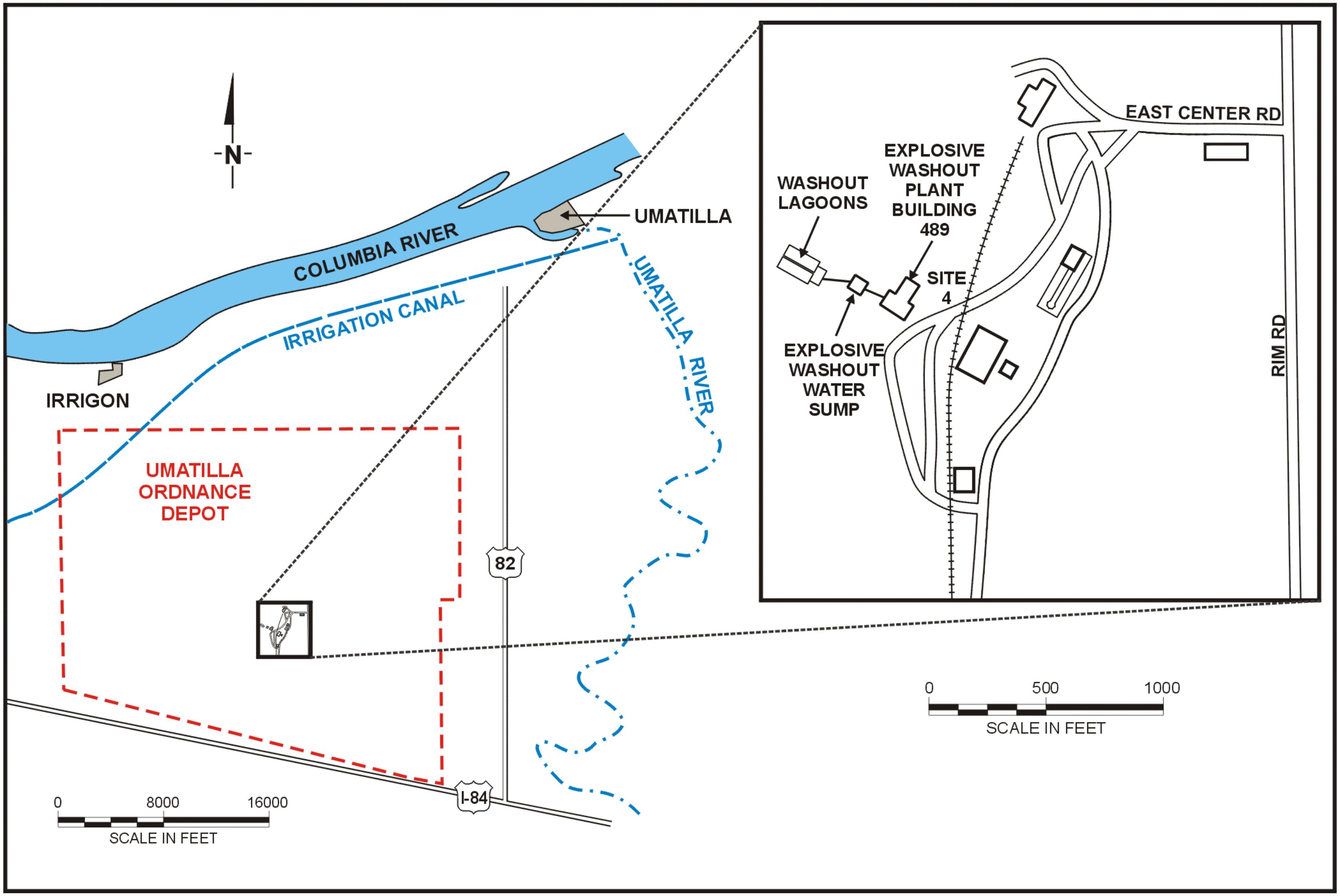


Figure 3-2. Site Location Map, Tooele Army Depot

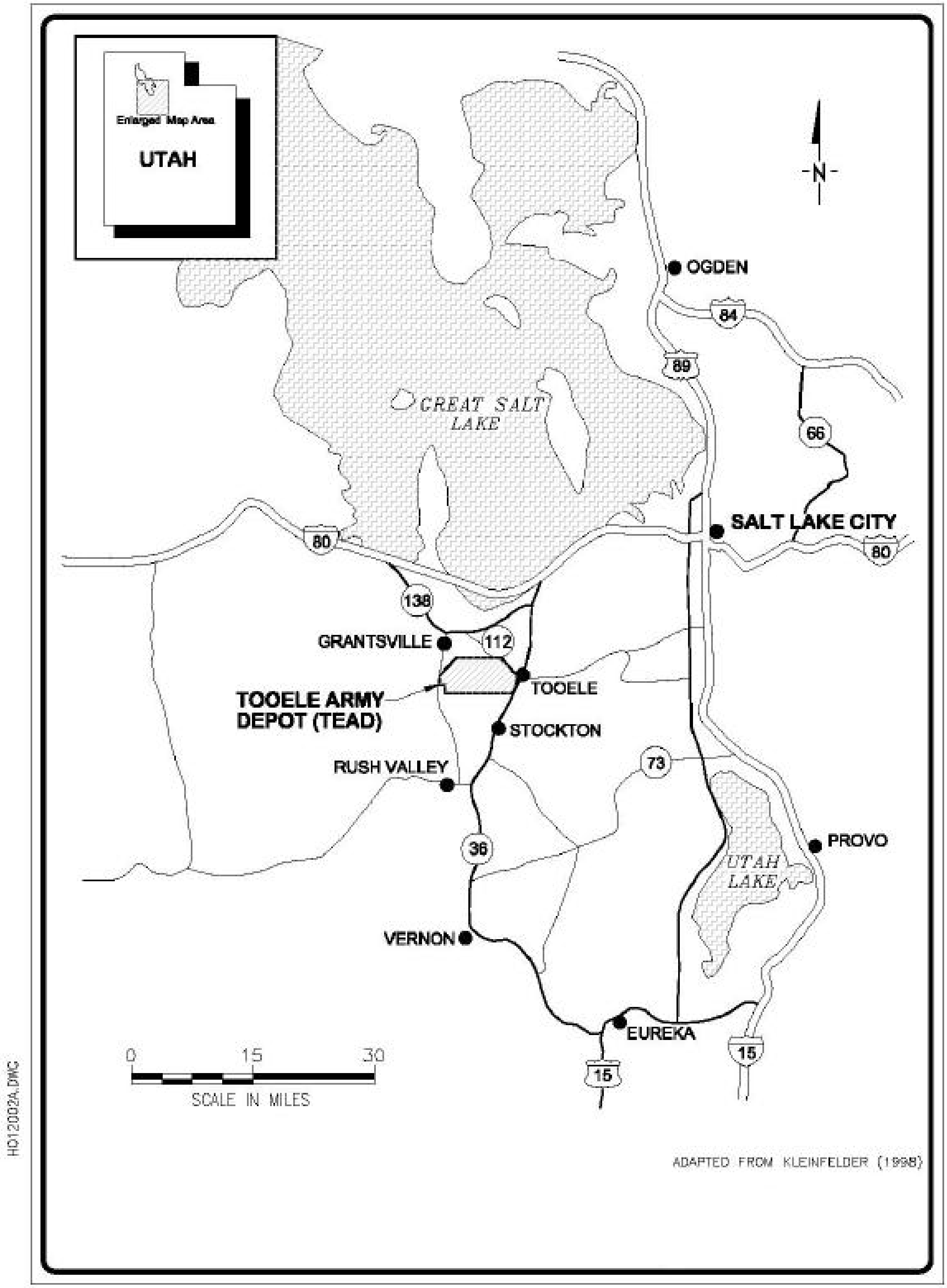


Figure 3-3. Site Location Map With TCE Distribution in Upper Semi-Confined Aquifer, Former Blaine Naval Ammunition Depot

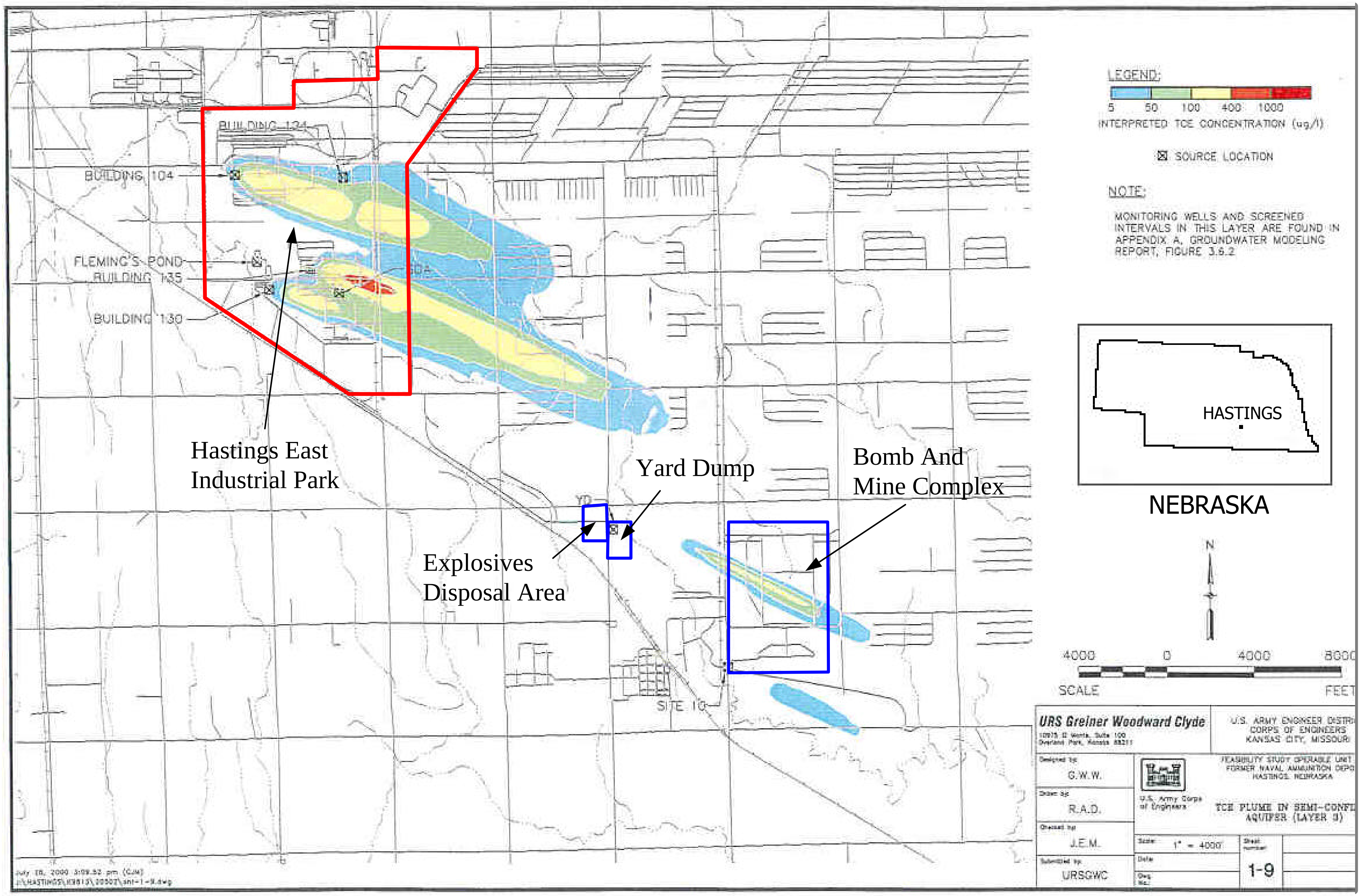


Figure 3-4. System Maps With Pre-Pumping RDX and TNT Plume Extents, Umatilla

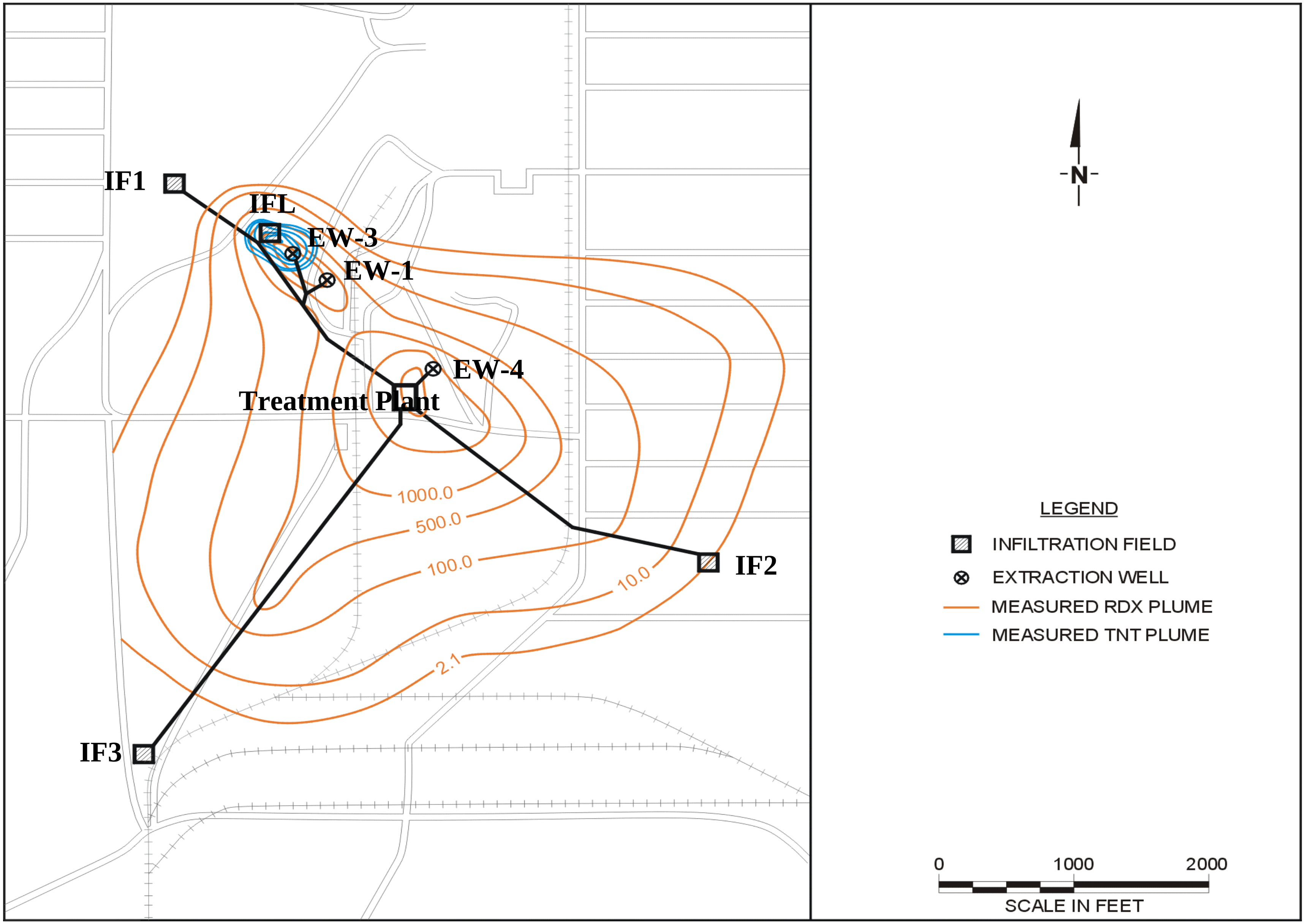
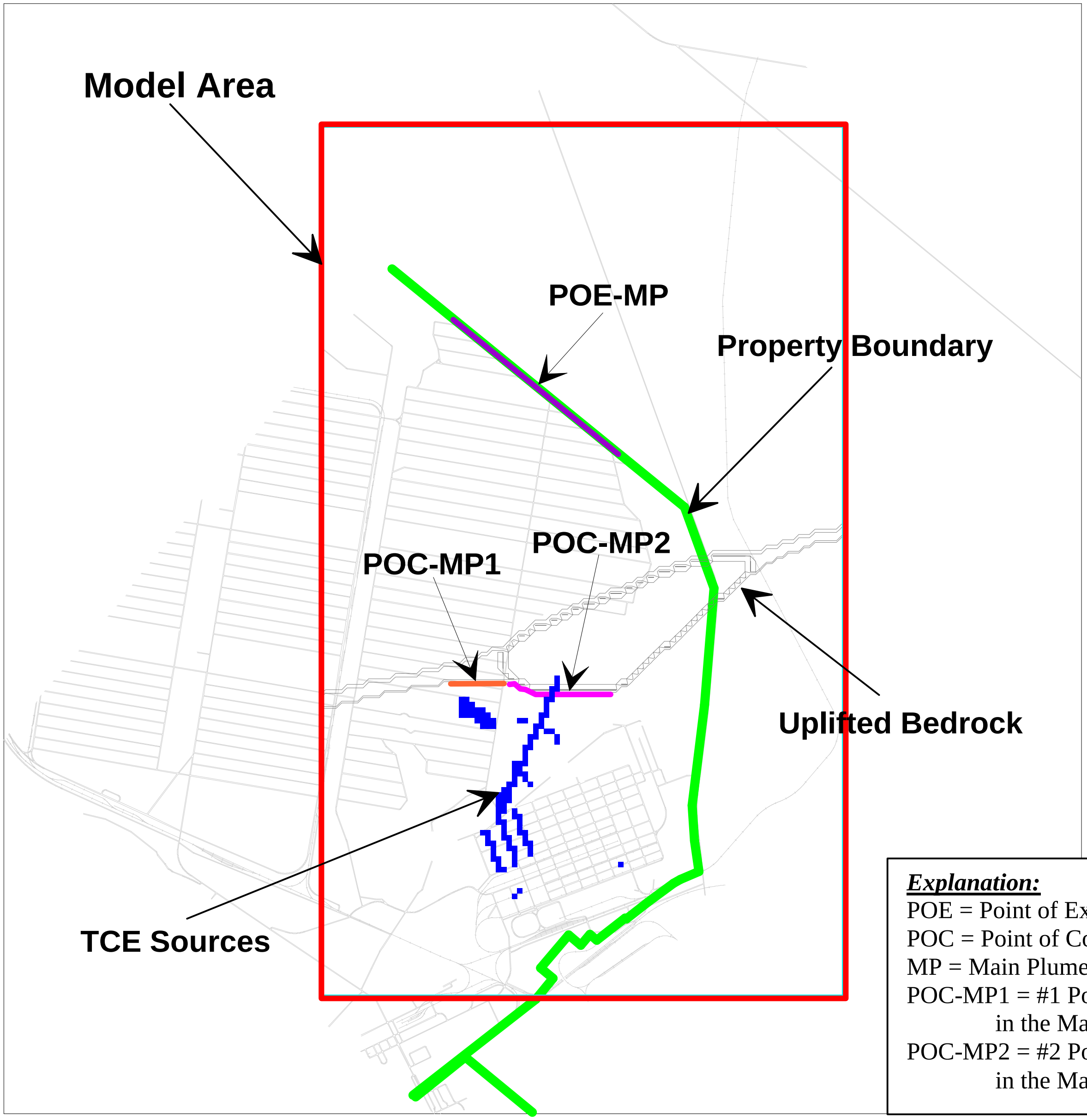


Figure 3-5. Site Map and TCE Sources, Tooele



Explanation:
POE = Point of Exposure;
POC = Point of Compliance;
MP = Main Plume;
POC-MP1 = #1 Point of Compliance in the Main Plume;
POC-MP2 = #2 Point of Compliance in the Main Plume

Figure 3-6. TCE Concentration In Model Layer 1 With System Configuration, End of Year 2002 (Initial Condition), Tooele

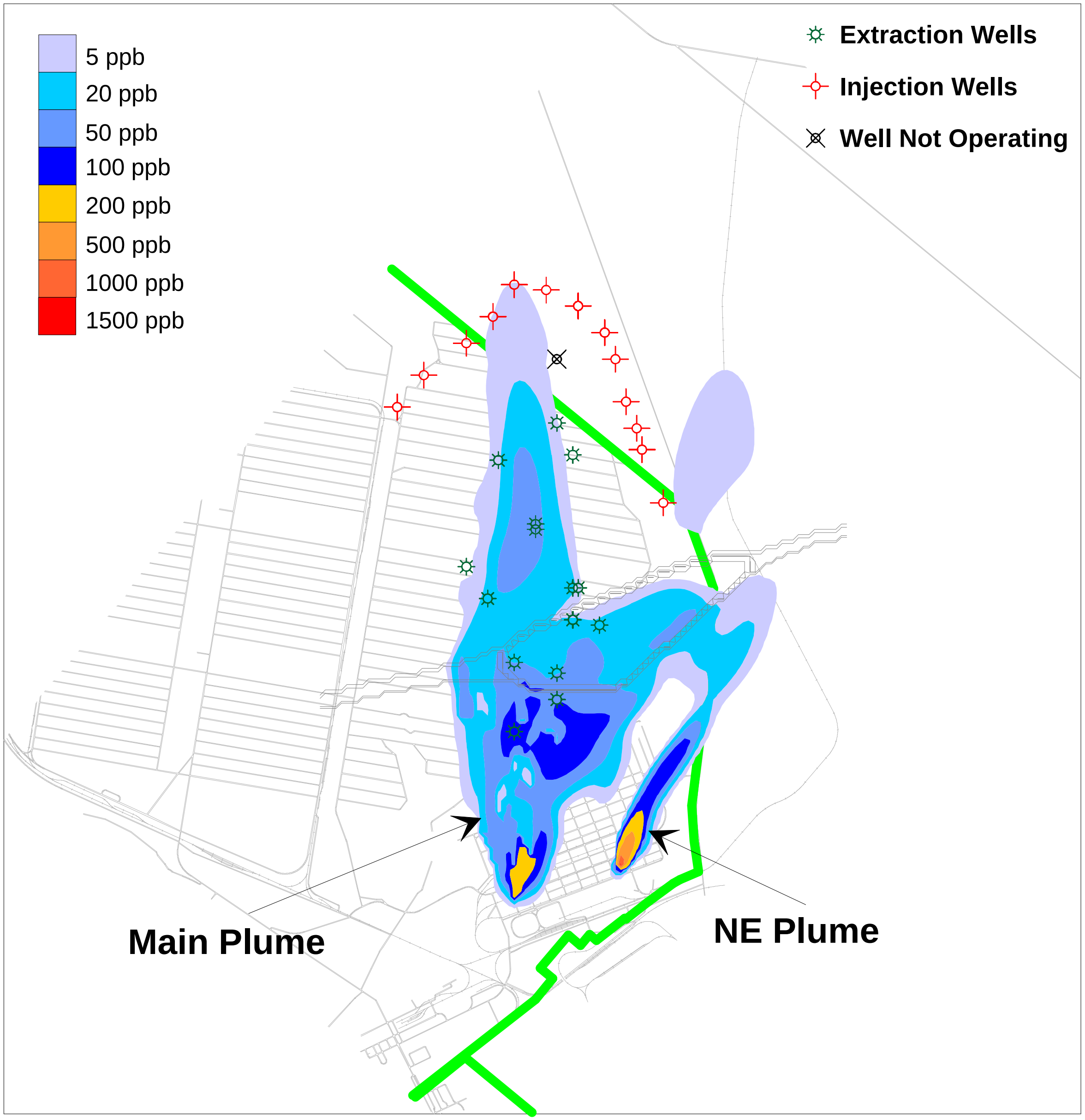


Figure 3-7. Commingled Plumes in Model Layer 1, 8/31/2002, Blaine

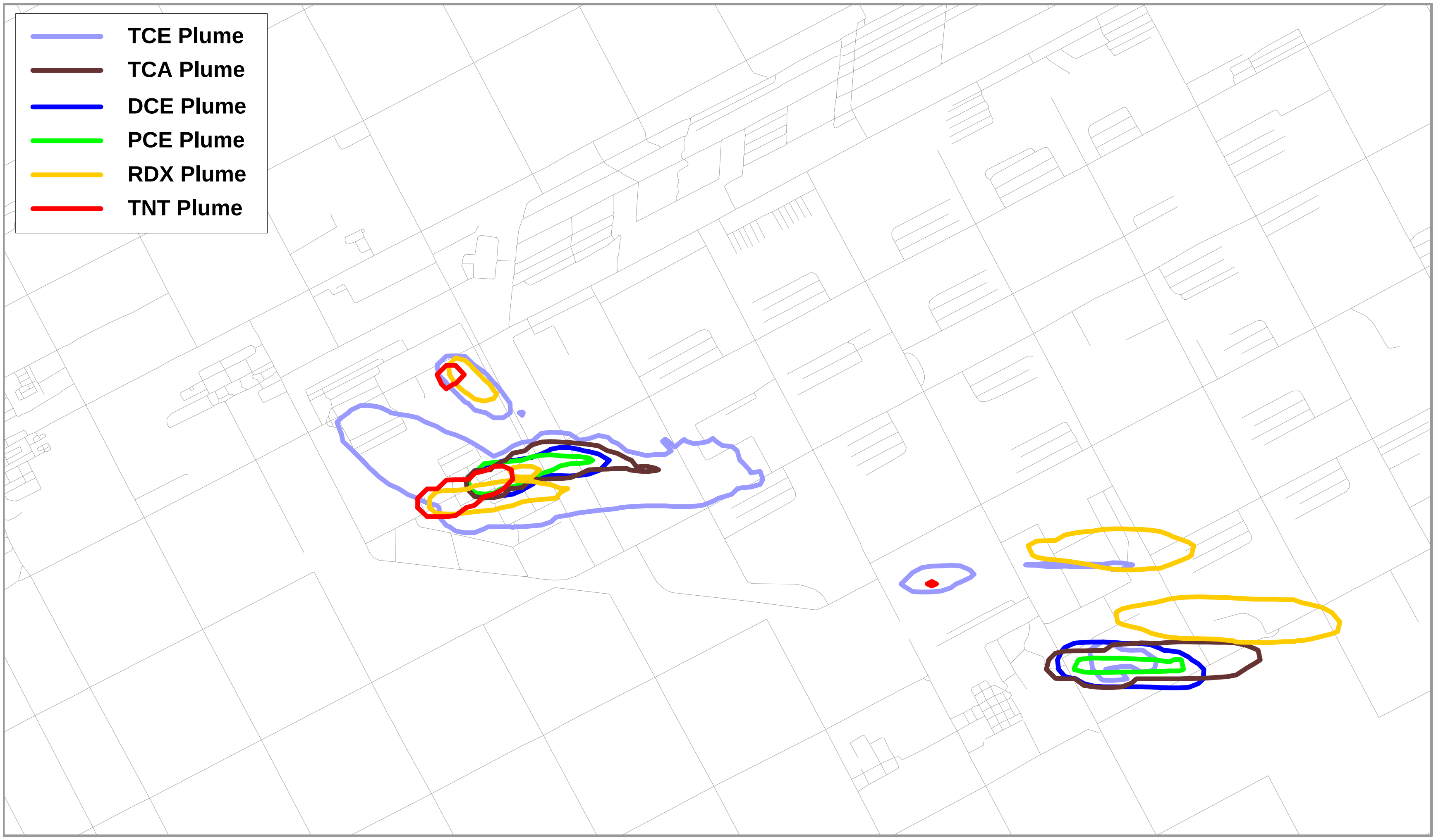


Figure 5-1. Cumulative Cost Over Time of Results Obtained by Three Groups, Umatilla Formulation 1

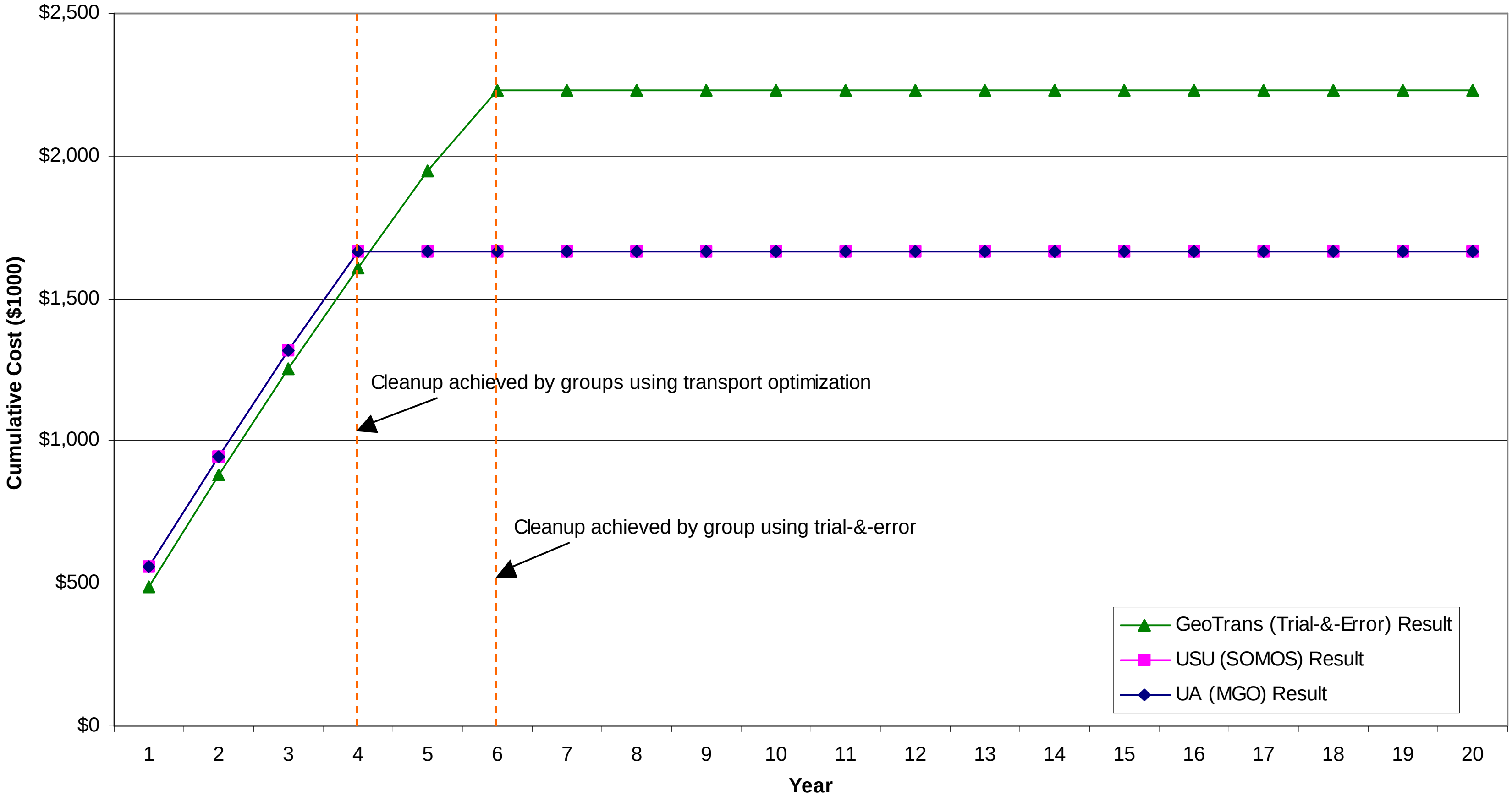


Figure 5-2. Hydraulic Conductivity Distribution in Model Layer 1, Umatilla

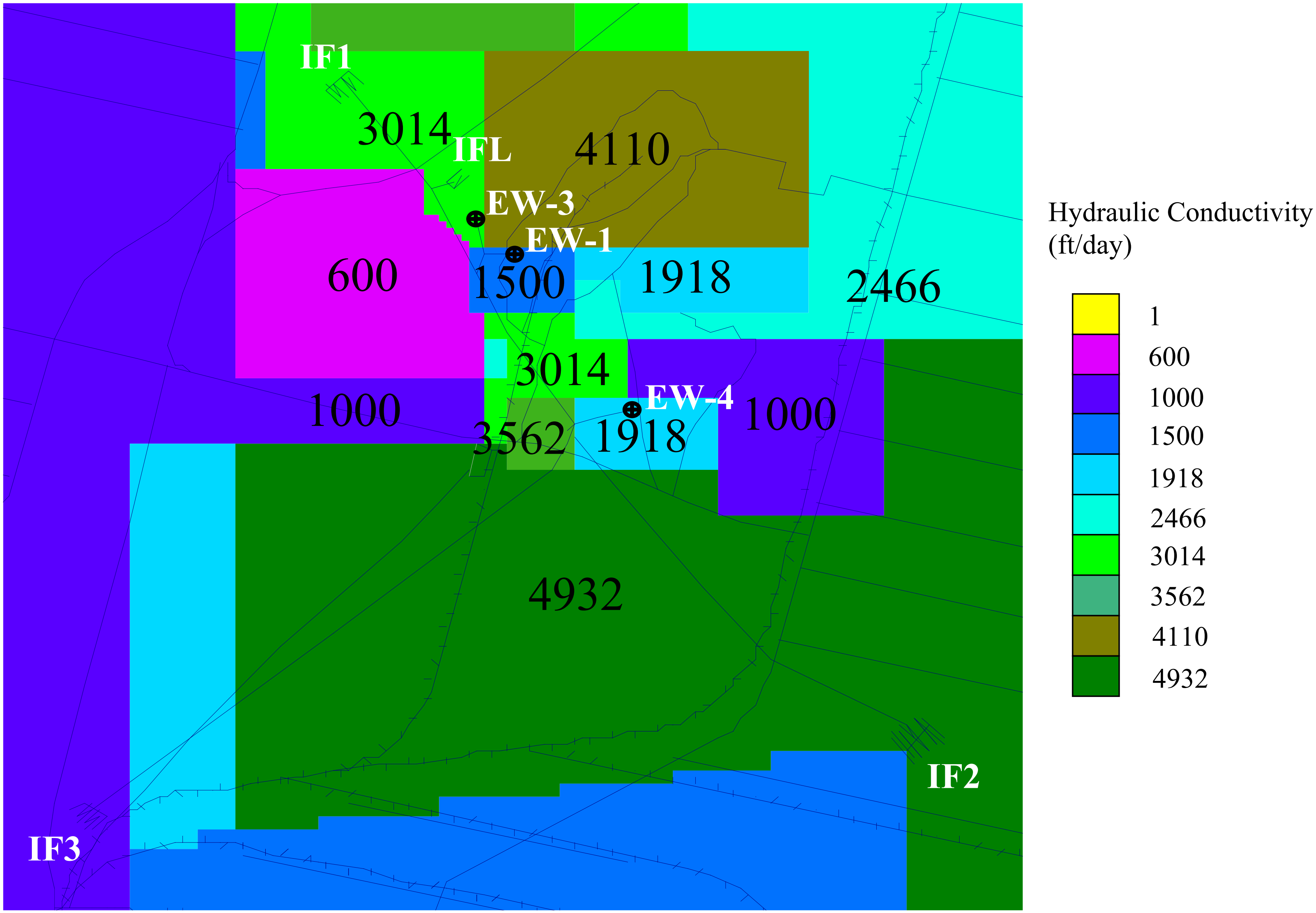


Figure 5-3. RDX Mass Remaining Over Time of Results Obtained by Three Groups in Model Layer 1, Umatilla Formulation 3

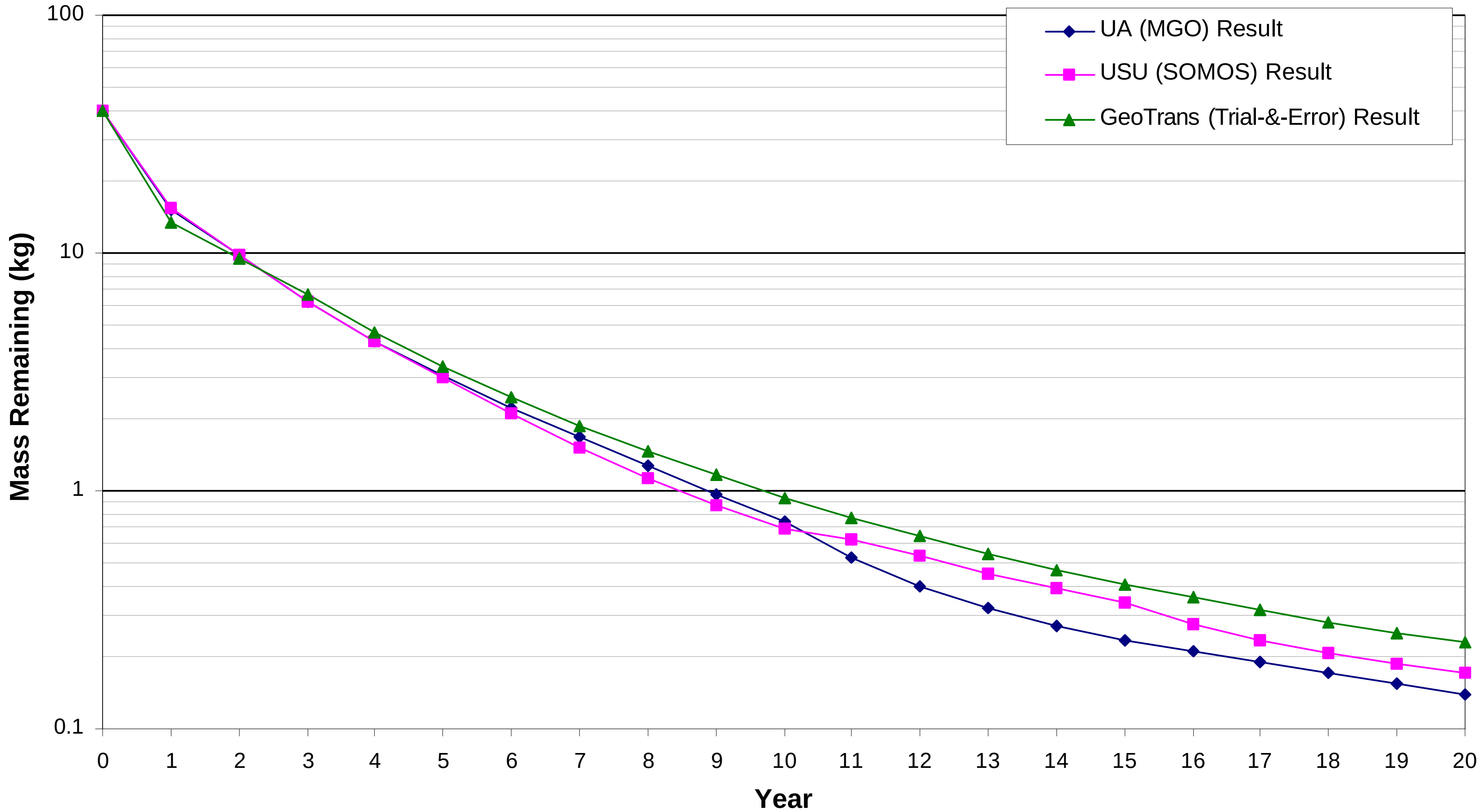


Figure 5-4. TNT Mass Remaining Over Time of Results Obtained by Three Groups in Model Layer 1, Umatilla Formulation 3

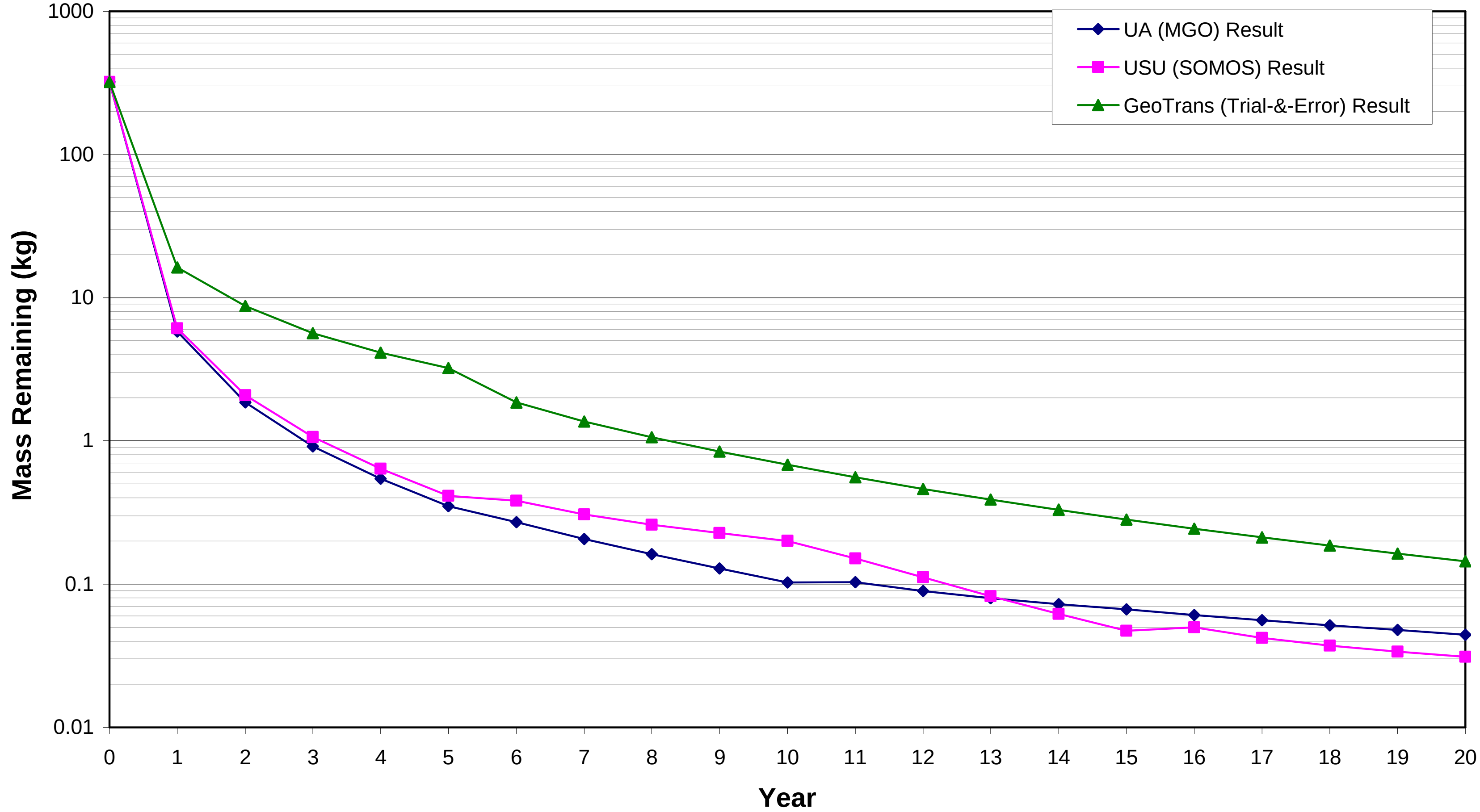


Figure 5-5. Cumulative Cost Over Time of Results Obtained by Three Groups, Tooele Formulation 1

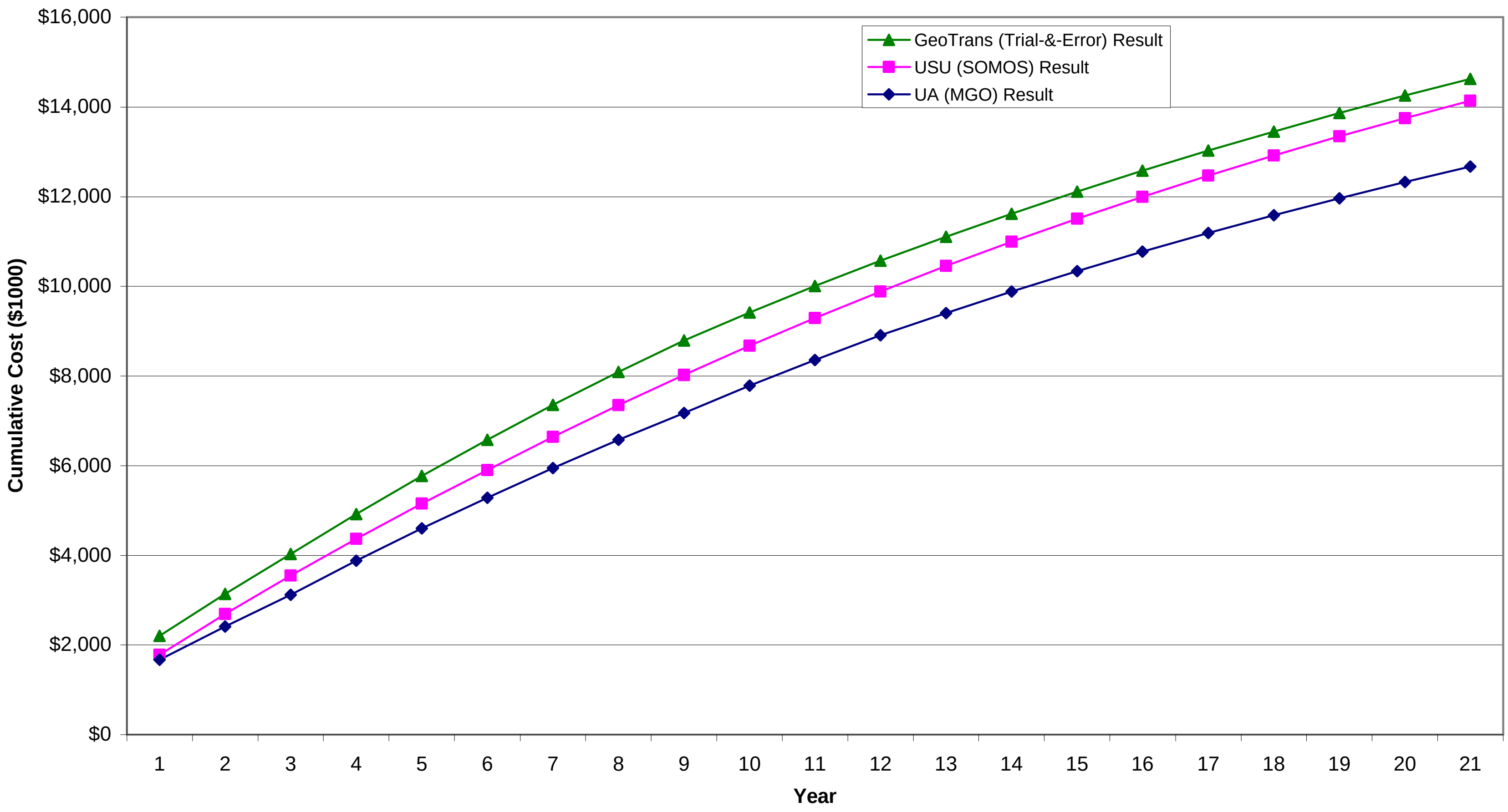


Figure 5-6. Cumulative Cost Over Time of Results Obtained by Three Groups, Blaine Formulation 1

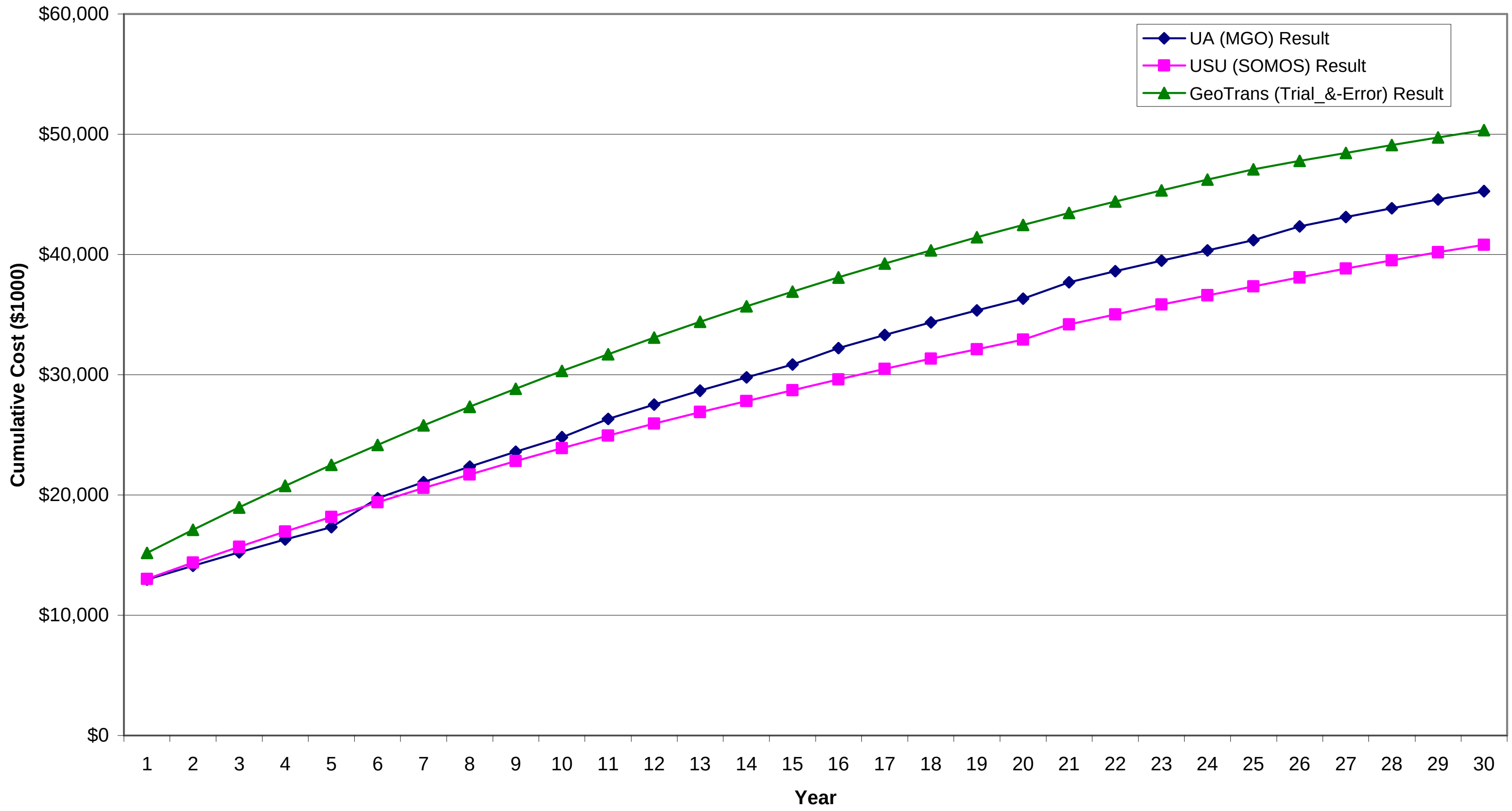
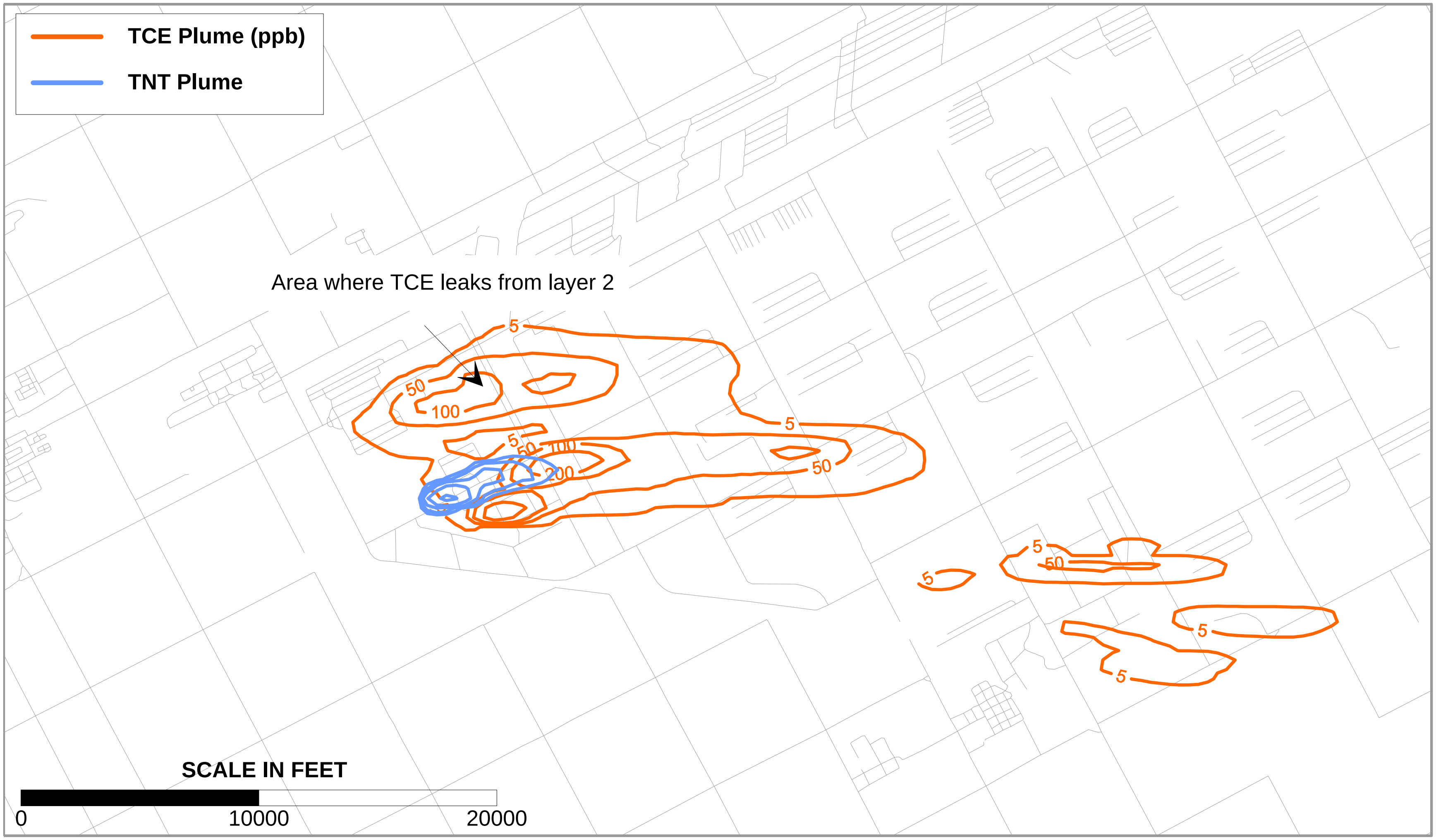


Figure 5-7. Simulated TCE and TNT Plumes, 8/31/2002, Model Layer 3, Blaine



APPENDICES

Appendix A: Points of Contact

Contact	Organization, Name, and Address	Phone/Fax/Email	Role in Project
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Appendix B: Phase 2 Demonstration Plan

ENVIRONMENTAL SECURITY TECHNOLOGY CERTIFICATION PROGRAM

DEMONSTRATION PLAN

FOR

APPLICATION OF FLOW AND TRANSPORT OPTIMIZATION CODES TO GROUNDWATER PUMP AND TREAT SYSTEMS

PART II: DEMONSTRATION OF TRANSPORT OPTIMIZATION CODES

JANUARY 2001

PREPARED BY NFESC AND HSI GEOTRANS

Table of Contents

Table of Tables

Table of Figures

Acronyms and Abbreviations

DCE	dichloroethylene
DoD	Department of Defense
EPA-TIO	Environmental Protection Agency Technology Innovation Office
ESTCP	Environmental Security Technology Certification Program
EW	extraction wells
FS	feasibility study
FY	fiscal year
GAC	granular activated carbon
gpm	gallons per minute
H	high
L	low
M	medium
NPV	net present value
O & M	operating and maintenance
PC	personal computer
ppb	parts per billion
RDX	royal demolition explosive
RI	remedial investigation
SVE	soil vapor extraction
TCE	trichloroethylene
TNT	trinitrotoluene
μg/l	micrograms per liter

1. Introduction

1.1 Background Information

The 1998 the Department of Defense (DoD) Inspector General report indicates that the cumulative operating and maintenance (O&M) costs for 75 pump and treat systems operating at DoD chlorinated solvent groundwater sites (a subset of over 200 DoD pump and treat sites) was $40 million in fiscal year (FY) 1996. The report also projected that these costs would reach $1 billion by the year 2020. Recent studies completed by the EPA and the Navy indicate that the majority of pump and treat systems are not operating as designed, have unachievable or undefined goals, and have not been optimized since installation. Even under ideal circumstances, (i.e., when the initial pump and treat system has been appropriately designed with clearly-defined objectives), changes in contaminant distributions and aquifer stresses, coupled with evolving regulatory climates result in the need for system optimization.

Although it is recognized that many of these pump and treat systems are ineffective for cleanup, regulations require that they continue to operate until a more effective solution is developed. In the interim, the potential for tremendous cost savings exists with the application of simple screening tools and optimization-simulation modeling. The optimization-simulation models link mathematical optimization techniques with simulations of groundwater flow and/or solute transport, to determine the best combination of well locations and pumping rates. Table 1, below, lists the DoD requirements for innovative pump and treat technologies.

Table 1. DoD Requirements for Innovative Pump and Treat Technologies

Service	Requirement Number	Requirement Title	Priority H,M,L
Army	A(1.5.o)	Development of Predictability Model for In-Situ Groundwater Treatment (Containment-Movement)	L
Air Force	2008	Methods and Remedial Techniques are Needed to More Effectively Treat Groundwater Contaminated with Chlorinated Solvents	M
Navy	1.I.1.e	Improved remediation of groundwater contaminated with non-chlorinated hydrocarbons	M
Navy	1.I.1.g	Improved remediation of groundwater contaminated with chlorinated hydrocarbons and other organics	H
Navy	1.II.1.a	Improved fate, effects and transport model for groundwater	M

1.2 Objectives of the Demonstration

The objective of this project is to demonstrate the cost benefit of applying transport optimization codes, which couple sophisticated optimization techniques (nonlinear programming) with simulations of groundwater solute transport, to existing pump and treat systems.

A previous project, which was sponsored by the US EPA (US EPA, 1999a,b) demonstrated potential avoidance of millions of dollars in O&M costs over the projected lifetime of the pump and treat system at two of three sites through the application of hydraulic optimization. Hydraulic optimization couples simpler optimization techniques (linear and mixed-integer programming) with simulations of groundwater flow (but not transport). Transport optimization techniques are potentially more powerful than hydraulic optimization techniques, because they not only look at optimization to accomplish hydraulic containment of the contaminant, but also to reduce contaminant concentrations to reach a desired cleanup goal. However, transport optimization codes are also more complex than hydraulic optimization codes.

This demonstration project is divided into two phases. Phase 1 is pre-optimization site screening and Phase 2 is the demonstration of transport optimization codes. The first Demonstration Plan (Part 1), prepared for this project in April 2000, addressed the development and application of a pre-optimization site screening methodology. The objective of the methodology is to prioritize sites on the basis of optimization potential, in terms of potential cost savings likely to result from an optimization-simulation evaluation. Eleven existing pump and treat systems at DoD installations will be utilized for this effort. (The criteria used to select these eleven sites are discussed in Section 3.1.) The resulting screening methodology will be a valuable tool for determining the potential cost savings from hydraulic and/or transport optimization at other DoD facilities.

This document describes the demonstration of transport optimization codes, which will be applied at three pump and treat sites. The demonstration will use existing groundwater flow and transport models for each site. A pre-requisite of selecting a site for the transport optimization simulations is that they have an existing transport model that they consider to be "up-to-date and acceptable for design purposes", based on previous conceptual model development and model calibration activities (which are specifically not within the scope of this project because this project is intended to evaluate the optimization algorithms and not the quality of the underlying transport models). An additional pre-requisite of selecting a site for the transport optimization simulations is an expression of willingness on the part of the installation to consider implementing recommendations that arise from the optimization results. The optimization formulations to be pursued at each site will be based on feasibility and usefulness as determined by the installation; however, it will be the responsibility of the installations to approach their regulatory agents if adjustments are desired. Although the installation is not bound per se to ultimately implement the recommendations, the project team will assist the installation during the implementation stage (if requested) in the form of additional presentations or more detailed descriptions of optimization results to the installation and/or regulators, and/or consultation with the installation regarding recommendations for any additional modeling or optimization simulations they may consider beyond the work performed during this project. Actual modifications to the pump-and-treat

system are not within the scope of this project, and would be the responsibility of the installation. However, tracking such modifications will be performed within the scope of this project.

1.3 Regulatory Drivers

There are no regulatory issues that will need to be directly addressed beyond those that have constrained the design and operation of the pump and treat systems being examined. Site personnel will be responsible for keeping their regulators involved in the project. However the ESTCP project team will encourage regulatory participation in the process and help site personnel communicate with their regulatory partners.

1.4 Stakeholder/End-User Issues

This demonstration is designed to address stakeholder and/or end-user decision factors concerning the implementation of optimization codes. In addition to evaluating the cost-benefit of applying optimization codes to flow and transport models, the demonstration will provide end-users with a pre-optimization screening tool to help determine if optimization codes will be cost-effective at particular sites. It is anticipated that this demonstration will provide end-users with the information to help them decide what level of optimization modeling (e.g. trial and error, hydraulic optimization, or transport optimization) is appropriate for their sites.

2. Technology Description

2.1 Technology Development and Applications

This project will demonstrate the utility of transport optimization codes for optimizing contaminant extraction rates and extraction well locations. Flow and transport optimization codes are algorithms that are attached to existing groundwater models to determine an optimal set of extraction and injection rates based on an objective function (to be minimized or maximized) and a set of constraints. Optimization will potentially result in reduced time and/or life cycle costs of pump and treat systems.

Most pump and treat systems have been designed through the use of flow or hydraulic numerical simulation models, such as MODFLOW 96. Traditionally, the hydraulic simulation model is run repeatedly to simulate different pumping scenarios. Each scenario is typically evaluated with respect to the number of wells required and the total pumping rate necessary to achieve the required hydraulic containment, while maintaining compliance with other design constraints (e.g., limits on water levels, drawdowns, etc.). These traditional, or manually iterative, simulations rely heavily on the experience and insight of the modeler, who must personally provide the adjustment, or incremental step towards optimization, for each successive trial. A limitation of this manually iterative approach is that there could be an infinite number of well locations and well rates, whereas only a small number of numerical simulations are practical.

Hydraulic optimization is an attractive alternative to the traditional modeling approach because computer programs can systematically evaluate a much greater number of possible combinations of well locations and pumping rates with respect to an objective function (e.g., "minimize total pumping rate") and a set of constraints. However, hydraulic optimization is limited by the underlying groundwater flow model's inability to predict contaminant concentrations. At sites where prediction of contaminant concentrations is crucial for designing the pump and treat system, transport simulation models can be applied. Transport models generally incorporate hydraulic or flow equations along with equations for contaminant partitioning, sorption and transformation, making them useful for prediction of cleanup times and/or compliance with concentration limits. Transport optimization codes are similar to hydraulic optimization codes, in that they allow a systematic evaluation of potential pumping strategies (i.e. using mathematical algorithms instead of manual iteration). However, optimization-simulation techniques incorporating transport simulations are significantly more complicated and computationally demanding than hydraulic optimization analyses.

The benefits of optimization-simulation modeling generally increase as the number of potential well locations increases. Similarly, the benefits typically increase as the total pumping rate of the pump and treat system increases. Optimization-simulation models can be applied with a variety of objective functions and constraints to efficiently evaluate different remediation strategies. For example, a modeler can evaluate system performance using minimum pumping rates for existing well locations, and subsequently evaluate the same system for a scenario with additional well locations. In contrast, this approach is much more difficult when performing simulations using

manual iteration. Similar limitations are observed for a related experimental strategy that is conducted empirically, i.e., by modifying a field variable and observing the effect with field measurements. The effectiveness of an empirical trial and error approach is restricted both by the number of alternatives that can be evaluated, as well as by the time and cost required for conducting the experiments. Thus, the application of optimization-simulation codes greatly enhances the scope of the problem that can be evaluated, and the efficiency with which potential solutions can be evaluated.

Optimization codes utilize two sets of variables for a pump and treat system optimization problem, decision variables and state variables. The most common decision variables are the extraction or injection rates of wells, well locations, and on/off status of particular wells. These decision variables can be specified or managed to identify their best or optimal combination. The state variables are hydraulic head and solute concentration, which are the dependent variables in the flow and transport equations. The optimization codes are coupled simulation-optimization models that determine the optimal values for all the decision variables (i.e. extraction/injection rates, well locations, etc.) based on simulations of the state variables.

Constraints are limits on the decision and/or state variables that are considered within the optimization problem. Examples of these constraints are: Limits on the extraction/injection rates, limits on well locations, limits on the number of wells, requirements that hydraulic heads be maintained above or below certain levels, or requirements that contaminant concentrations don't exceed regulatory standards at points of compliance. The coupled simulation-optimization approach is appealing because it can account for the complex behavior of the groundwater flow system and identify the best optimization strategy given the cleanup objectives and constraints.

There are many optimization solution techniques. Some of the classical approaches include linear programming, non-linear programming, mixed integer linear programming, mixed integer non-linear programming, and differential dynamic programming. Recently, a new class of optimization methods referred to as "global optimization methods" has emerged. These include simulated annealing, artificial neural networks, genetic algorithms, outer approximation, and tabu search. These global methods are being used more and more, despite their requirement for intensive computational efforts. For this ESTCP demonstration, the transport optimization modelers will select the best methods based on site specific requirements and their specific expertise.

2.2 Previous Testing of the Technology

Since the 1980's, many researchers have sought to couple groundwater simulation models with mathematical optimization techniques to address groundwater management issues. In 1999, the Environmental Protection Agency Technology Innovation Office (EPA-TIO) conducted a hydraulic optimization demonstration at three pump and treat sites using the MODMAN hydraulic optimization code. Optimization strategies for two of the three sites suggest potential life cycle cost avoidance in millions of dollars. The MODMAN code has been available and in use by consultants in commercial projects for over 5 years. The most recent version (Version 4.0) developed for the EPA will soon be available for free from an EPA website. In addition, the EPA-TIO demonstration developed a pre-optimization screening tool that was used and will be

revised for this demonstration. Transport optimization codes are more developmental in nature. Several universities have developed transport optimization codes, and some have been tested at sites. Three examples of recent applications of transport optimization are provided below.

Chemical Spill-10 (CS-10) site located at the Massachusetts Military Reservation

Two of the three recent applications of Transport optimization were applied at this site. A pump and treat system is operating to remediate and contain a TCE plume approximately 17,000 feet long, 6,000 feet wide, and up to 140 feet thick. Between Fall 1999 and Spring 2000, transport simulation-optimization codes were utilized to maximize TCE mass removal over a 30-year time horizon, subject to the following constraints: (1) the TCE concentration must be lower than or equal to 5 ppb beyond the base boundary, (2) all extracted water must be reinjected into infiltration trenches, (3) individual wells are subject to pumping capacities, and (4) the total pumping rate should be restricted for cost considerations. The decision variables were the extraction rates and well locations for four perimeter wells that were being considered, and the extraction rates for five in-plume wells that were already constructed.

University of Alabama - Dr. Chunmiao Zheng

In this case (AFCEE, 1999), the optimal strategy, as determined by the simulation-optimization analyses, suggests using only one perimeter well (rather than four wells) and a maximum pumping rate of 2700 gallons per minute (gpm). The results of the analysis demonstrate that it possible to remove more TCE mass (approximately 3.5%) under the same amount of pumping assumed in the trial and error design, and that it can also lead to substantial cost savings by reducing the number of wells needed and adapting dynamic pumping. Preliminary cost estimates indicated that this strategy would yield life cycle cost savings of $2.4 million.

Utah State University - Dr. Richard Peralta

In this case (Peralta et al, 1999a, b), the simulation-optimization modeling enhanced mass removal rates and aided in well placement. Specifically, the modeling identified a configuration that would extract approximately 6% more mass over 30 years, while reducing the extraction rate by 50 gpm.

A third recent application:

Wurtsmith Air Force Base, MI: Optimizing Contaminant Mass Removal Using Artificial Neural Network. Waterstone, Inc. - Dr. Alaa Aly

In this case (Aly, A.H. and R.C. Peralta 1999a), optimization codes were used to develop an optimal strategy for remediating TCE and DCE groundwater plumes. Management goals and restrictions were identified and prioritized as follows:

- Capture the TCE and DCE dissolved phase groundwater plumes
- Reduce TCE and DCE concentrations to < 94 ppb and < 230 ppb, respectively, within 6 years
- Total extraction of groundwater cannot exceed 400 gpm
- No treated water may be injected into the groundwater

- Treatment facility effluent cannot exceed 5 ppb of TCE

An artificial neural network was used to simulate contaminant concentrations in the optimization model. The model considered a total of 24 potential extraction well locations. Six alternative optimal pumping strategies were ultimately evaluated for the final design. After discussions with stakeholders, a final strategy was chosen based on its minimization of total pumping rates, minimization of total time to meet objectives, and overall benefit to the stakeholders.

2.3 Factors Affecting Cost and Performance

This demonstration project will rely heavily on the existing information at the selected pump and treat sites, particularly the existing flow and transport models. There may be some additional costs involved if existing models require minor updates or calibration. The results of the optimization modeling will be based on the information existing in the current models.

2.4 Advantages and Limitations of Transport Optimization Codes

A properly defined optimization problem can be solved through manual trial and error adjustment or using a formal optimization technique. While the trial and error method is simple and widely used, testing and checking hundreds or thousands of trial solutions is tedious, time consuming, and cannot guarantee that the optimal solution will be identified. Transport optimization codes can be used to identify the optimal solution and, equally important, to prove whether a particular optimization strategy is feasible and will satisfy all constraints.

Key advantages of transport optimization codes include:

- they are automated and repeatable,
- many combinations of extraction and injection well rates can be evaluated,
- they are unbiased by historical events, and
- they quickly solve modified problems.

Limitations of transport optimization codes include:

- the complexity of the algorithms require specialized modelers for optimization,
- the codes may require high powered computers to complete optimization runs, and
- the results from these codes are only as accurate as the existing groundwater predictions.

3. Demonstration Design

3.1 Performance Objectives

The performance objective of this project is to demonstrate the cost benefit of applying transport optimization codes to existing pump and treat systems, which have been pre-screened for optimization potential. The cost benefit will be evaluated by analyzing the performance of a currently operating pump and treat system after application of:

1. transport optimization codes (innovative technology), and
2. traditional, manually iterative optimization methods (baseline alternate technology). These traditional methods, which will be performed independently, rely heavily upon the experience and insight of the modeler, who must personally provide the adjustment, or incremental step towards optimization, for each successive trial. The traditional approach may incorporate hydraulic optimization codes to solve surrogate optimization problems based only on groundwater flow components.

Note that the specific performance objectives will be identified for each site based on interaction with the installation. Some performance objectives listed in Table 2 (e.g., faster remediation) may not be specifically evaluated at one or more of the demonstration sites. This cost benefit evaluation will be performed at three separate pump and treat sites.

Table 2. Performance Objectives

Type of Performance Objective	Primary Performance Criteria	Expected Performance (Metric)	Performance Objective Met?
Qualitative	1. Reduce annual operating costs	Annual operating costs less than current costs	
	2. Faster remediation	Increased contaminant removal efficiency compared to current efficiency	
	3. Reduce cost of system life cycle	Reduced annual cost and/or reduced expected operating time	
Quantitative	1. Reduce annual operating costs	> 20%	
	2. Reduce system life cycle costs	> 20%	

3.2 Selecting Sites

The site screening process is discussed in detail in *Technology Demonstration Plan for Application of Flow and Transport Optimization Codes to Groundwater Pump and Treat Systems, Part 1: Pre-Optimization Screening* (hereafter referred to as Part 1 TDP). A brief description of the process follows.

The site selection process consists of three steps: (1) Gather data on existing DoD pump and treat systems, (2) Screen DoD systems with a series of "kick out" questions to narrow the list to eleven potential demonstration sites, and (3) Apply further pre-optimization screening to select three appropriate demonstration sites.

Members of the project team conducted phone interviews to identify candidate pump and treat sites within the DoD. Sites were first screened to meet the following set of criteria:

- Total pumping rate is at least 50 gpm
- A flow model is documented, and is considered up-to-date and valid for design purposes by the Site and the regulators, and
- A transport model is documented, and is considered up-to-date and valid for design purposes by Site and the regulators (or it is considered realistic that the transport model can be completed, documented and considered valid for design purposes by Site and regulators within six months of selection for transport optimization).

The criteria for minimum total pumping and minimum annual O&M cost eliminate sites with limited opportunity for significant cost savings using a transport optimization approach. The criteria pertaining to the existence of adequate flow and transport models eliminate sites for which a subsequent transport optimization analysis would not be possible within the time frame of this demonstration project.

After the initial screening process to identify potential sites, more detailed information was collected for each site (see Section 5.2 of Part 1 TDP) and the following criteria were applied to select candidate sites:

- Annual O&M costs at least $100K/yr
- Time horizon for pump and treat system operation is at least 5 years
- Pump and treat system is operating or in final design stage
- Up-to-date plume maps for key contaminants exist, and
- Interest in participating on this project.

In addition, the selection of the eleven sites incorporates the following preferences pertaining to the existing models:

- simple to moderate complexity is preferred (e.g., more than 10 model layers, if actually required to provide adequate simulation, is probably too complex for this study)
- a single-phase, porous-media model simulating flow/transport in the saturated zone is preferred (i.e., multi-phase codes and/or saturated/unsaturated codes and/or specialized

fracture-flow codes are more complex, subject to greater uncertainty, and generally require more simulation time than is appropriate for this demonstration project)

These preferences eliminate excessively complex sites, which would prevent the timely completion of the subsequent transport optimization simulations, and/or obscure the discussion of the case study in the final report. Table 3 provides a list of the eleven sites selected for pre-optimization screening.

Table 3. Candidate Sites for Pre-Optimization

Facility/Site	Flowrate (gpm)
Tooele Army Depot, UT	7000
Cornhusker Army Ammunition Plant, NE	600
Umatilla Army Depot, OR	1300
Shaw Air Force Base, SC	250-300
McClellan Air Force Base, CA	1100-1200
Wurtsmith Air Force Base, MI	750
George Air Force Base, CA	5-6 (upper aquifer) 100 (lower aquifer)
Wright-Patterson Air Force Base, OH	400-600
Naval Air Engineering Station Lakehurst, NJ	500
Marine Corps Air Station Cherry Point, NC	90
Marine Corps Air Station Yuma, AZ	200

The final step is to select three demonstration sites. The original plan for this project was to select three demonstration sites prior to beginning the optimization process. However, during the site selection process, the project team determined that it would be necessary to include the optimization modelers in the selection process. Their expertise should be utilized to evaluate groundwater models and other site-specific characteristics that might affect the application of optimization codes. Therefore, the first site will be selected with the help of the transport optimization modelers and demonstration will then commence at that site while the selection process for the second and third sites continues.

Detailed site information is required for the final site selection, including system operation and maintenance cost, the estimated cost for new extraction well and piping installation, existing

groundwater models, plume maps, site characterization information, and records of system performance. The existing groundwater models must be up to date and of sufficient quality or the site managers must be willing to update the models before the site can be considered for selection. Another major criterion for this demonstration is the willingness of site managers to fund the implementation of any optimization recommendations made for the site.

Of the eleven sites listed in Table 3, Tooele Army Depot, Cornhusker Army Ammunition Plant, Umatilla Army Depot, Shaw Air Force Base, McClellan Air Force Base, and Wright-Patterson Air Force Base show potential for cost savings and are being more thoroughly investigated as potential demonstration sites. Currently, the strongest candidate site is Umatilla Army Depot. Detailed site history and pump and treat operations information for Umatilla is presented in Sections 3.3 and 3.4 below.

3.3 Test Site History/Characteristics – Umatilla Chemical Depot, OR

3.3.1 Historical Background and Remedial Action/Remedial Design

Umatilla Chemical Depot is a 19,728-acre military reservation established in 1941 as an ordnance depot for storage and handling of munitions. The facility is located in northeastern Oregon straddling the border of the Umatilla and Morrow counties, three miles south of the Columbia River and six miles west of Hermiston, Oregon (Figure 1). Originally Umatilla's mission included the storage, renovation and demilitarizing of conventional munitions and storage of chemical munitions. In 1994, as a result of the Base Realignment and Closure (BRAC) Act, the depot's mission was changed to storing chemical munitions until their destruction under the Chemical Stockpile Disposal Program and site remediation.

From the 1950s until 1965, the depot operated an onsite explosives washout plant. The plant processed munitions to remove and recover explosives using a pressurized hot water system. The principal explosives included 2,4,6-Trinitrotoluene (TNT) and Hexahydro-1,3,5-trinitro-1,3,5-triazine (commonly referred to as Royal Demolition Explosive or RDX), Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (commonly referred to as High Melting Explosive or HMX), and 2,4,6-Tetranitro-N-methylaniline (Tetryl). In addition, the munitions contained small quantities of 2,4-Dinitrotoluene (2,4-DNT); 2,6-Dinitrotoluene (2,6-DNT); 1,3,5-Trinitrobenzene (TNB); 1,3-Dinitrobenzene (DNB); and nitrobenzene (NB), occurring as either impurities or degradation products of TNT (USACE 1998a).

The wash water from the plant was disposed in two unlined lagoons, located northwest of the plant, where wash water infiltrated into the soil. During the 15 years of operation of the washout plant, an estimated 85 million gallons of wash water were discharged to the lagoons. Although lagoon sludge was removed regularly during operation of the plant, explosives contained in the wash water migrated into the soil and groundwater at the site. The groundwater table is encountered approximately 47 feet below the lagoons. Because of the soil and groundwater contamination of the lagoons, the site was placed on EPA’s National Priorities List (NPL) in 1984.

The Army initiated a Remedial Investigation (RI) of the lagoons in 1987. The RI was used to identify the types, quantities, and locations of contaminants and to develop ways of addressing contamination (Dames & Moore 1992a).

Following the environmental investigation studies, a Human Health Baseline Risk Assessment (Dames & Moore 1992b) and a Feasibility Study (FS) (Arthur D. Little, Inc. 1993) were conducted. These evaluations were conducted to define remediation goals and criteria and to identify, evaluate, and provide the basis for selection of remediation alternatives for mitigating explosives contamination. The site was divided into Soils and Groundwater Operable Units, based on the independent methods for addressing those two avenues of public and worker exposure.

Upon review of the RI/FS, the US Army, US Environmental Protection Agency (EPA), and the Oregon Department of Environmental Quality selected a cleanup plan for the groundwater operable unit. As described in the Record of Decision (USACE 1994), Alternative 4B was selected. The major components of the alternative are:

- Pumping groundwater from extraction wells over an estimated 10 to 30 year period
- Treating extracted groundwater with granular activated carbon (GAC) to remove contaminants
- In-situ flushing of subsurface soils beneath the lagoons with all or part of the treated groundwater for an estimated period of one year
- Reinfiltration of the treated groundwater outside the contaminant plume
- Monitoring of groundwater contamination to determine the effectiveness of the remedial action and to determine when groundwater cleanup levels have been attained
- Institutional controls on the contaminated groundwater to prevent its use until cleanup levels are met
- Remediation of the groundwater is scheduled to continue until the concentration of explosives in the aquifer meets cleanup levels. The cleanup level for RDX is 2.1μg/l and TNT is 2.8 μg/l.

A groundwater treatment system was designed to implement Remediation Alternative 4B. Design of the groundwater treatment system was based in part on the results of model studies described in the Final Remedial Design Submittal (USACE, 1996). The remedial design configuration is shown in Figure 2. Groundwater remediation at the site began with official plant startup on 15 January 1997.

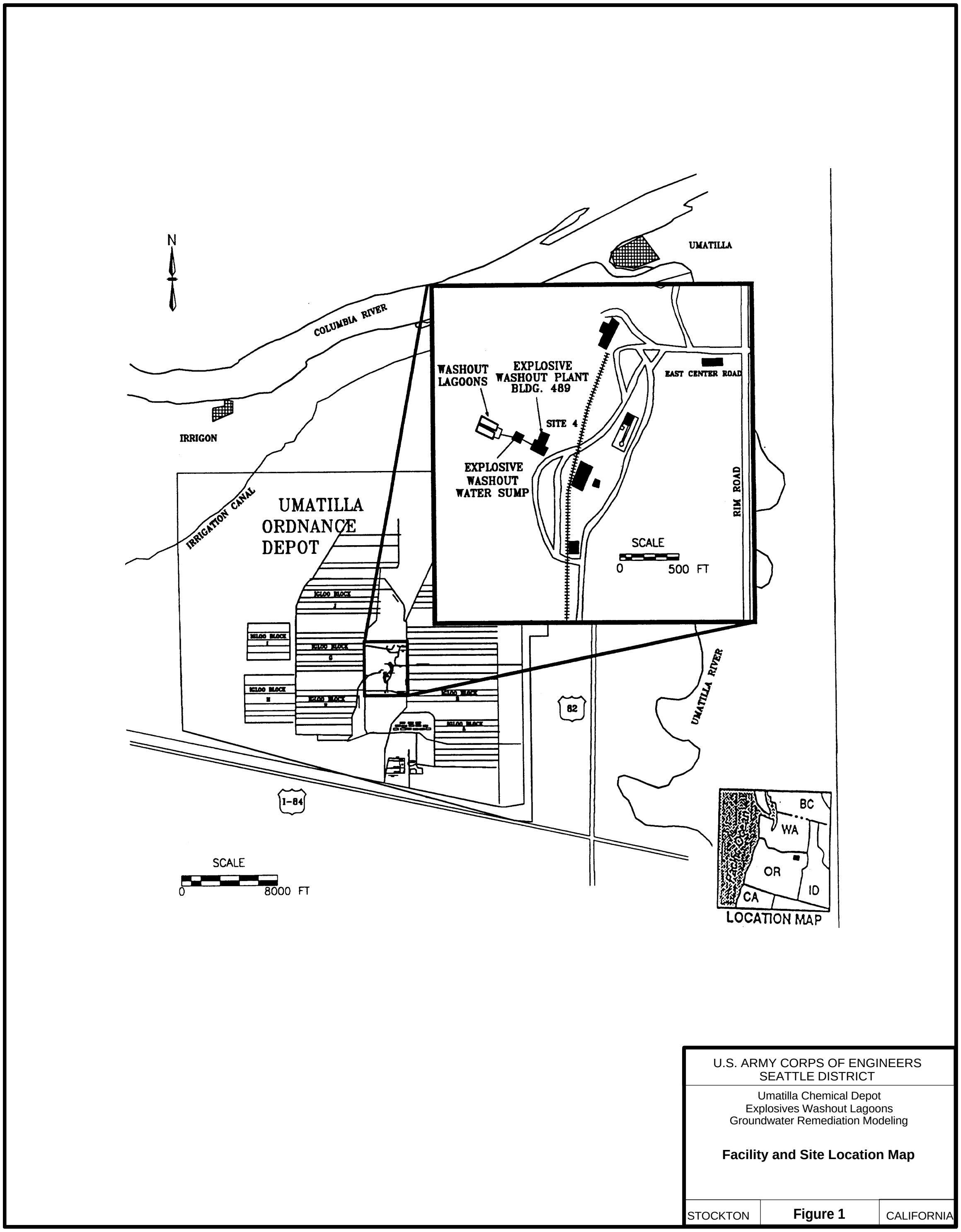

Figure 1. Facility and Site Location Map

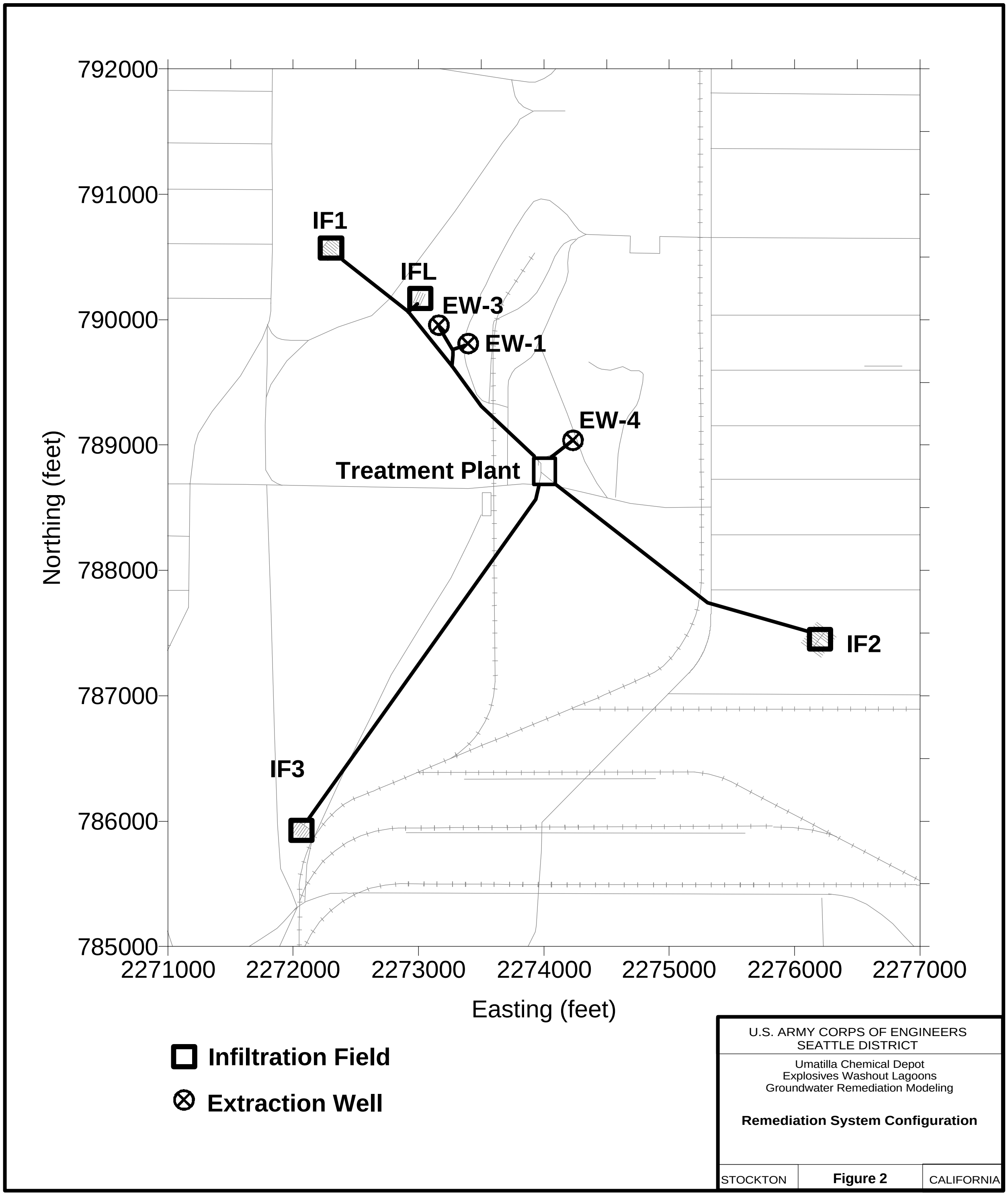

Figure 2. Remediation System Configuration

3.4 Present Operations – Umatilla Army Depot, OR

3.4.1 System Operations

The groundwater treatment system began extracting, treating and re-infiltrating contaminated groundwater on 15 January 1997. The system has operated since that time with the exception of an extended period of shutdown for treatment system adjustment during the first quarter of operation, intermittent power outages, and periodic treatment plant GAC replacement events. The total pumping rate vs. time for the period of 15 January 1997 through 15 July 1999 (first 2.5 years of operation) is shown in Figure 3. Umatilla estimates its current operation and maintenance costs as $400,000 per year and expects the site to close in approximately 13 years.

3.4.2 Contaminant Mass Removed

Approximately 1.27 billion gallons of contaminated groundwater was extracted from, treated and recharged to the aquifer by 15 July 1999. The mass of RDX and TNT removed from the aquifer during this time period was calculated using two data sets: field test analytical results of groundwater at the influent port to the treatment plant and fixed laboratory analytical results for water sampled from extraction wells. RDX mass removed is estimated at 3,442 and 3,741 kg using field and fixed lab data, respectively. TNT mass removed is estimated at 432 and 392 kg using field and fixed lab data, respectively.

3.4.3 Plume Reduction

The initial measured RDX plume present in the aquifer before system startup is shown in Figure 4. The measured RDX plume in July 1999 is shown in Figure 5. Significant retreat of the 2.1 μg/l contour has occurred between infiltration gallery 1 and the washout lagoons, along the western margin of the plume, and along the southern margin of the plume. To the north and northeast, the 2.1 μg/l plume boundary may have migrated outward due to infiltration from the washout lagoons. Concentrations of RDX have declined at all extraction and monitoring wells except for two wells located in the northern and northeastern portion of the plume.

The initial TNT plume measured in the aquifer before system startup is shown in Figure 6. The measured TNT plume in July 1999 is shown in Figure 7. The center of the TNT plume has migrated southeast toward EW-1 and the plume has grown larger. TNT migration and plume expansion is due to pumping at EW-1 and EW-4 and to infiltration at the lagoons.

The concentrations of RDX and TNT for the first 2.5 years of system operations for the extraction wells (EW-1, EW-3 and EW-4) are shown in Figures 8 and 9, respectively. RDX concentrations have generally declined with time at all extraction wells. A slight annual oscillation of concentration is due to the slight seasonal shifting of the plume due to regional groundwater gradient oscillations. RDX concentrations at EW-4 were relatively constant for the first 0.3 years and then increased slightly before beginning a steady downward trend. TNT concentrations at EW-4 have been consistently non-detect. TNT concentrations at EW-1 rose sharply as the center of the TNT plume shifted southeast in response to EW-1 and EW-4 pumping and lagoon infiltration.

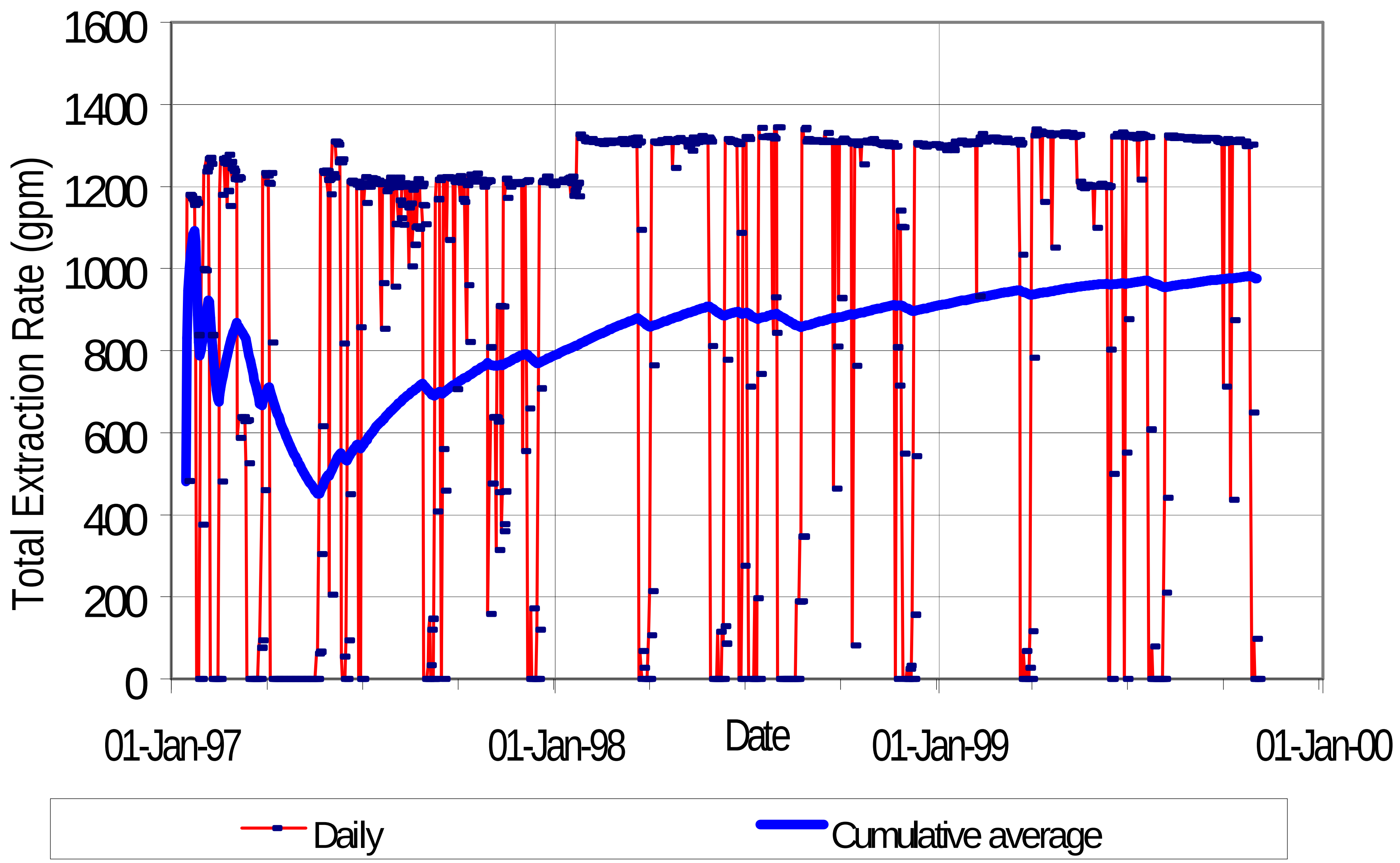

Figure 3. Total Pumping Rate versus Time – 15 January 1997 though 15 July 1999

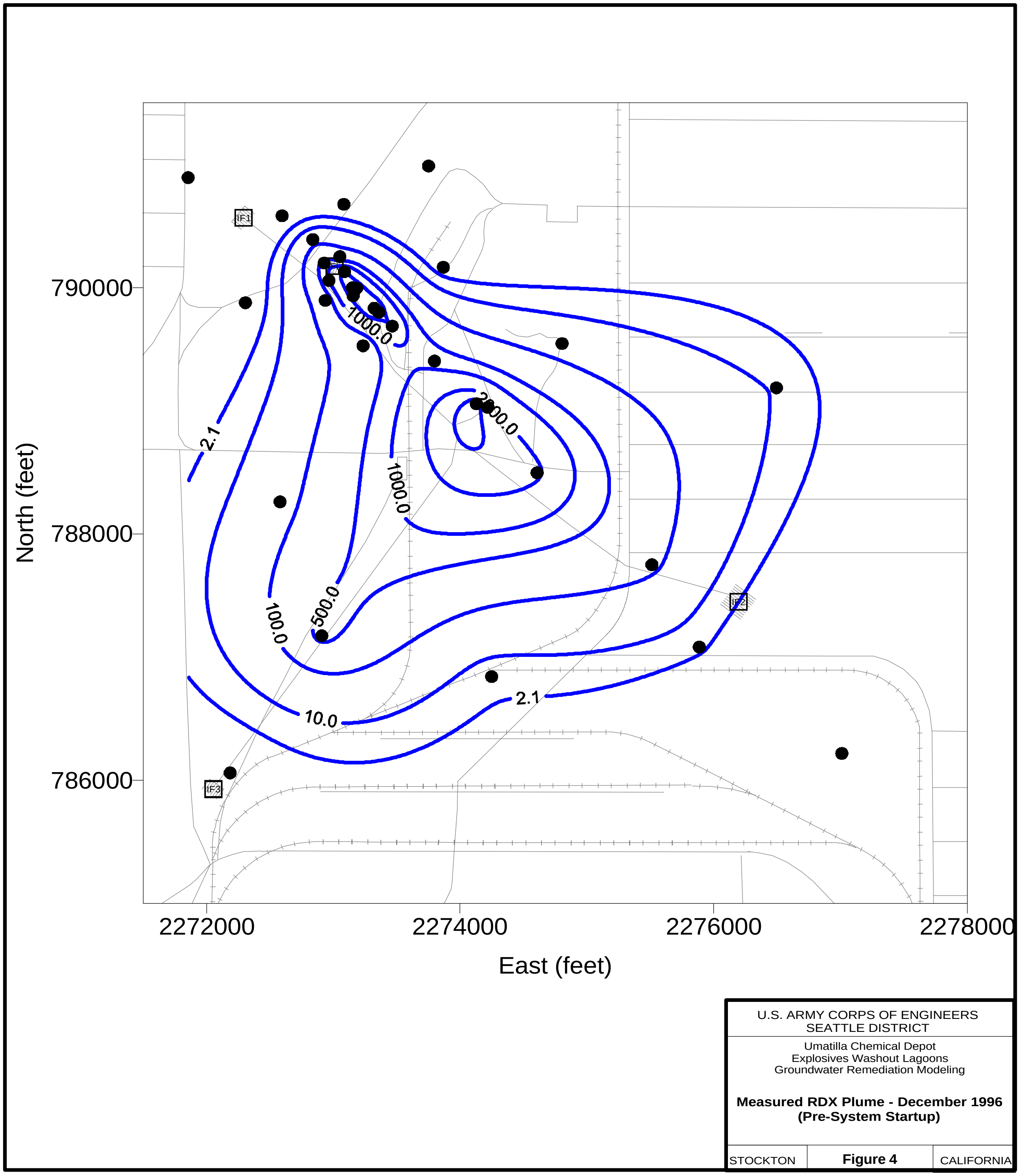

Figure 4. Measured RDX Plume – December 1998 (Before System Startup).

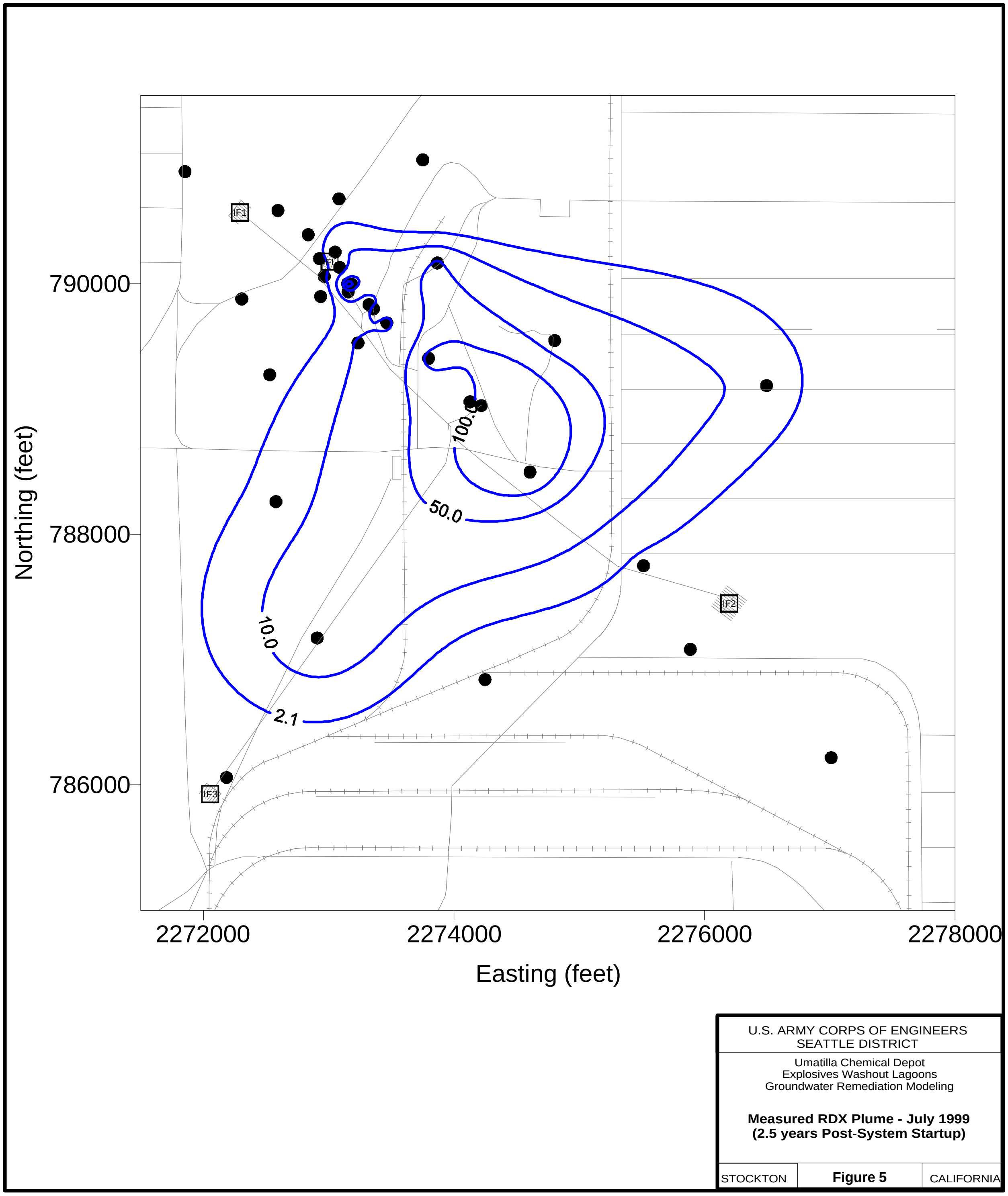

Figure 5. Measured RDX Plume – July 1999 (2.5 years After System Startup).

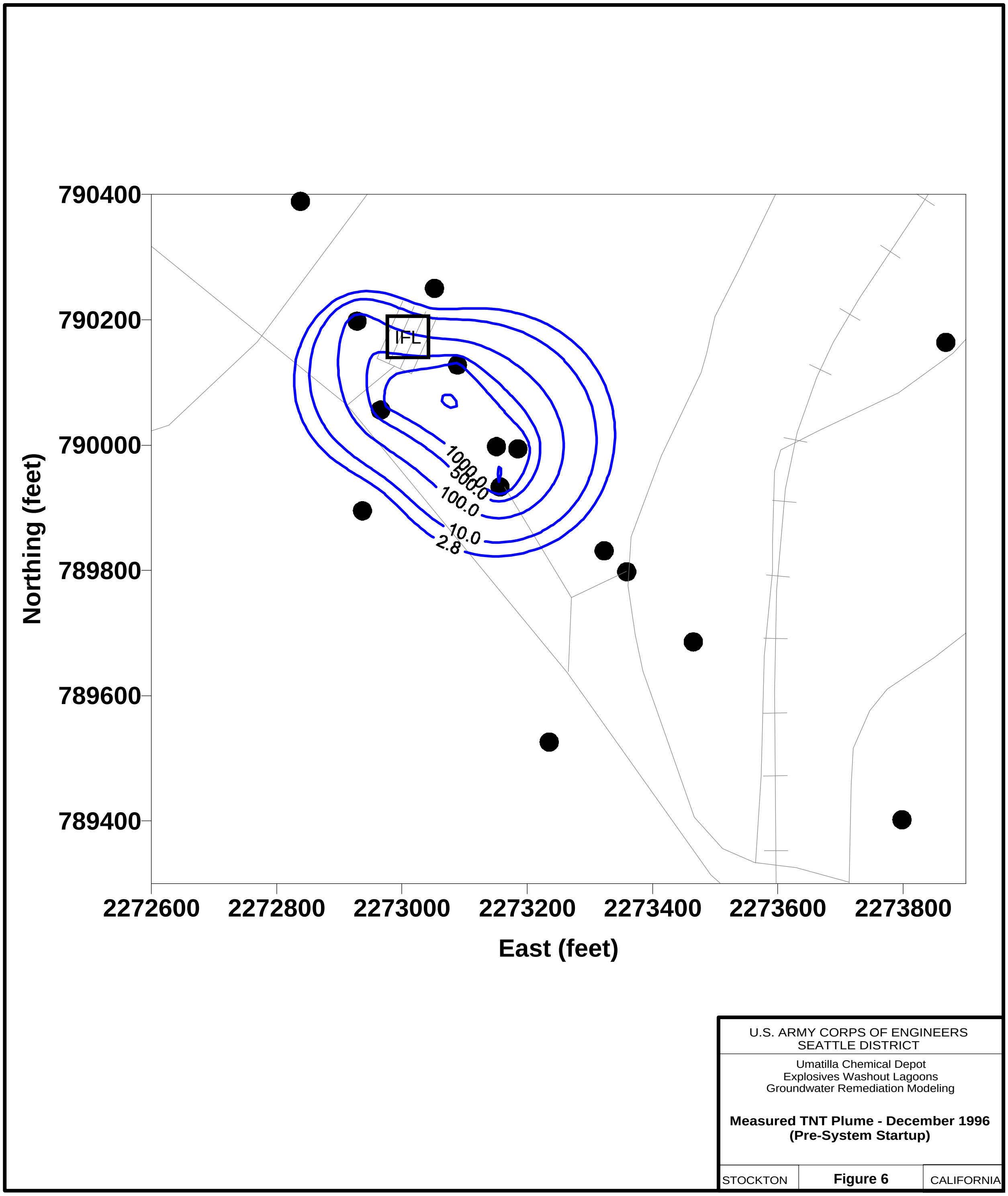

Figure 6. Measured TNT Plume – December 1996 (Before System Startup)

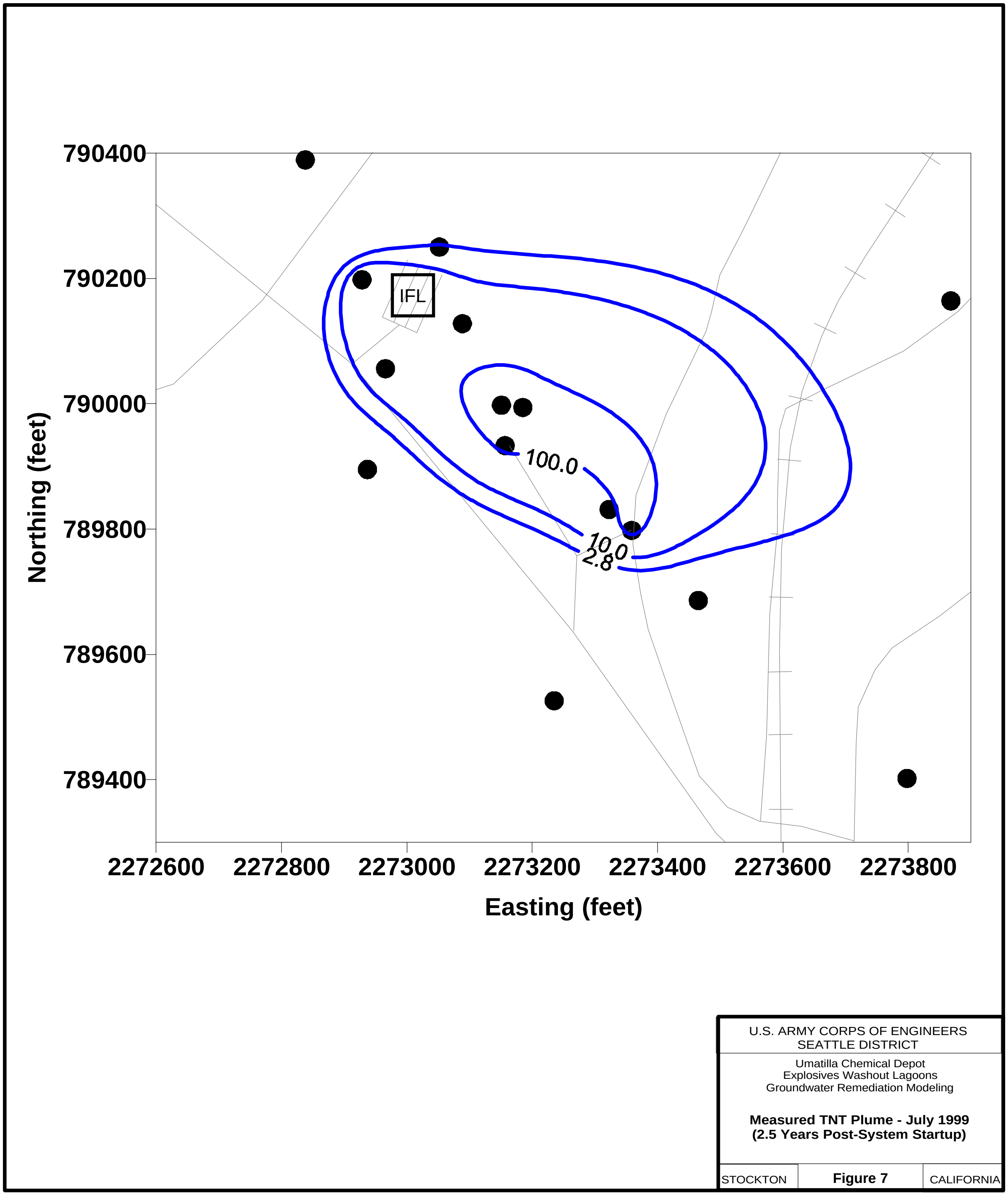

Figure 7. Measured TNT Plume – July 1999 (2.5 Years After System Startup).

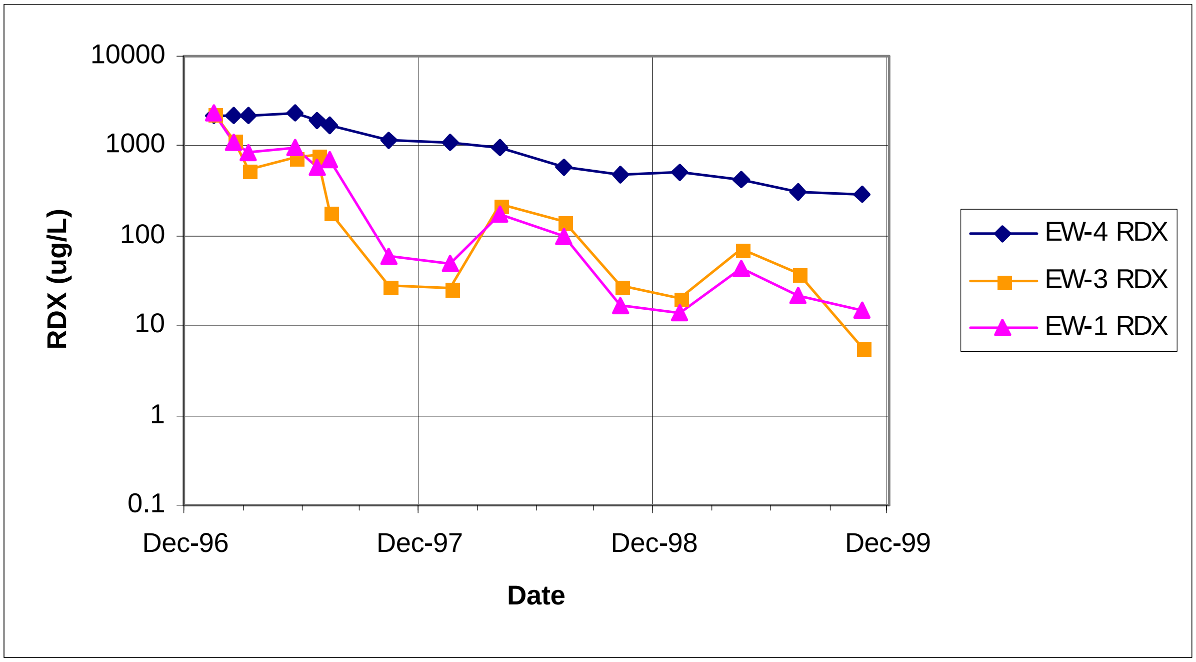

Figure 8. Concentration of RDX for First 2.5 Years of System Operation - Extraction Wells 1, 3 and 4.

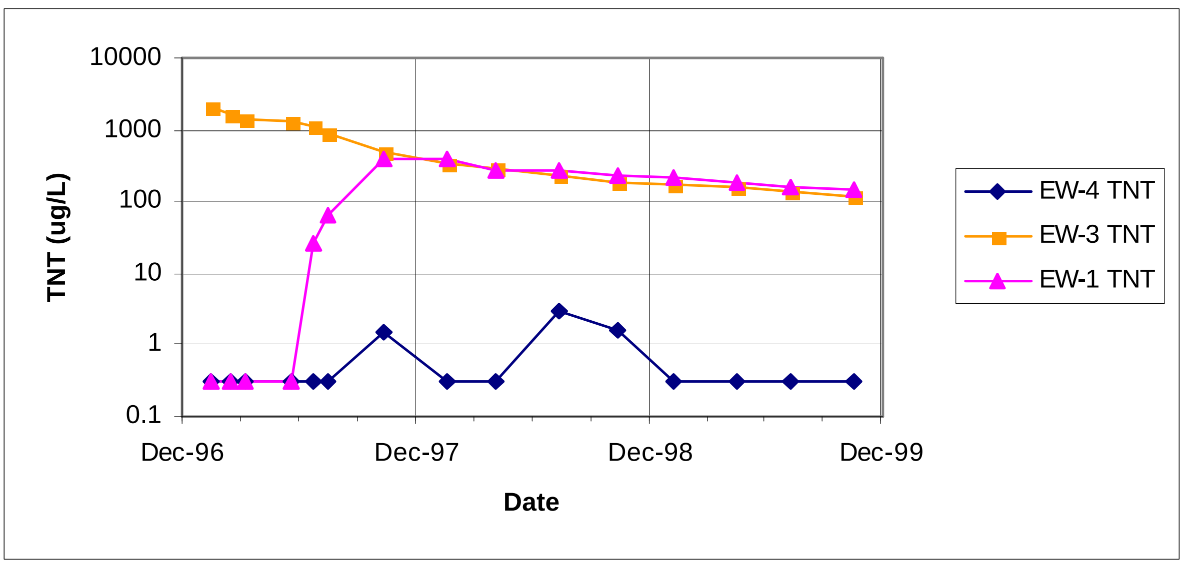

Figure 9. Concentration of TNT for First 2.5 Years of System Operation - Extraction Wells 1, 3 and 4.

3.4.4 Groundwater Elevation Data

The groundwater gradient in the vicinity of the explosives washout lagoon oscillates approximately 180 degrees in the absence of treatment system pumping and infiltration. Presumably, agricultural pumping causes the groundwater gradient in the alluvial aquifer to shift toward the south in the summer and fall, and recharge during the winter and spring causes the gradient to shift to the north. The design model did not simulate the seasonal variations in groundwater elevations or groundwater gradient. Instead, the model was calibrated to simulate the average yearly gradient. The average yearly gradient for the first year of operations is shown in Figure 10.

3.5 Pre-Demonstration Testing and Analysis

No groundwater sampling and analysis will be performed as part of this project. During the pre-optimization screening process, existing plume maps for key contaminants were compiled and evaluated to understand the prevailing or "baseline" contamination scenario. This was done to understand the remedial objectives. Confirmation was requested from the installation to establish that the plume maps represent the most current understanding of contaminant distribution for the site.

At most facilities with operating pump and treat systems, groundwater monitoring is conducted on a regular basis. This updated groundwater concentration data can be used to recalibrate the groundwater models, further characterize source areas, and alter remedial objectives. It will be necessary to establish a fixed set of plume maps and groundwater models to be used for the demonstration project. Prior to final site selection, the optimization modelers will evaluate the existing site characterization data and verify that the plumes have been delineated using the most recent monitoring data available. The modelers will also evaluate existing groundwater models to verify the input data sets are current and accurate. These data and models will be used as the baseline information for each site throughout the project for performance comparisons.

A large part of the pre-optimization screening is related to system operation costs. This project will utilize current costs associated with the operations of each system as the baseline for evaluating the optimization recommendations. The life cycle costs will be calculated for recommended optimization strategies and compared to the baseline costs.

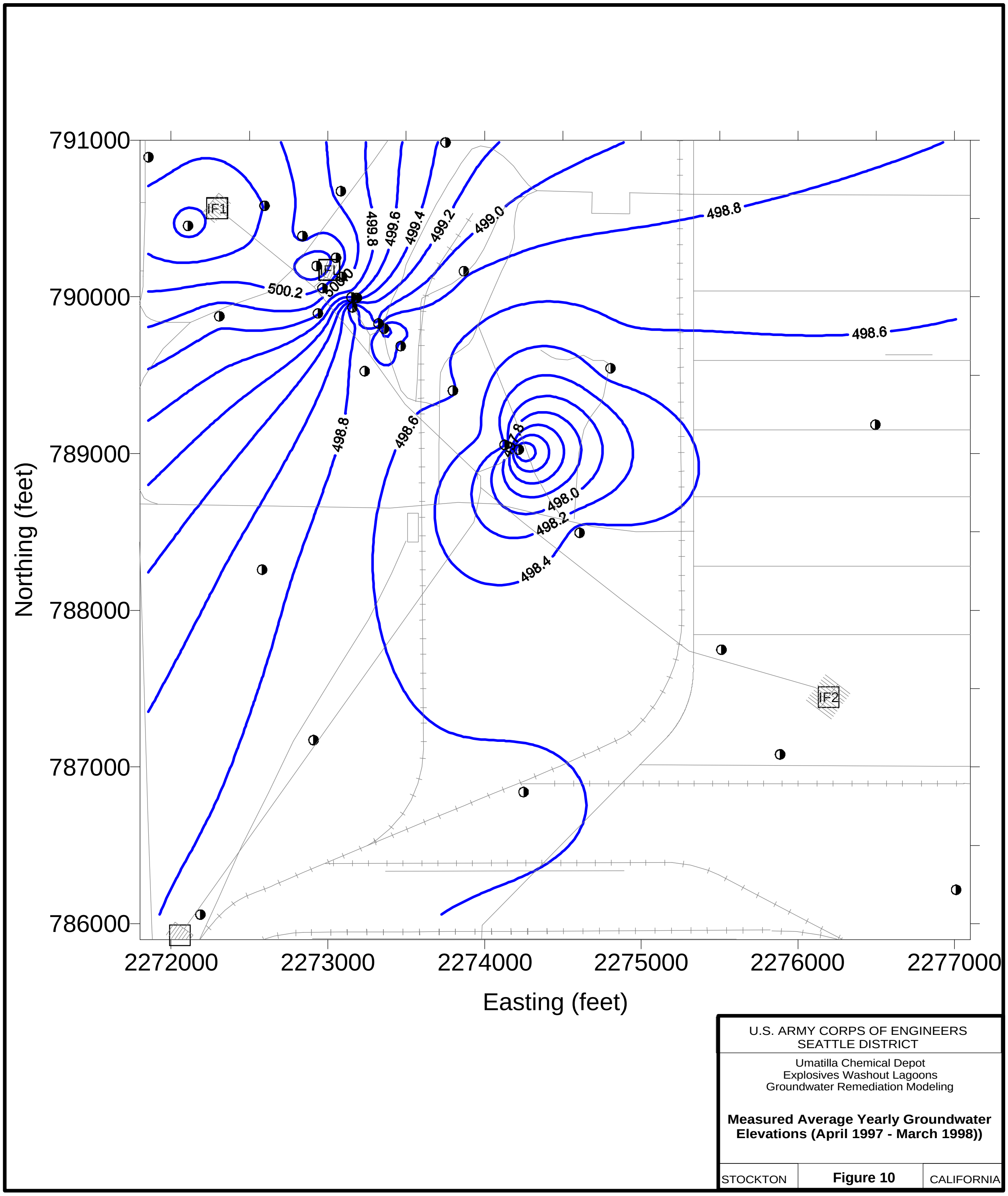

Figure 10. Measure Average Yearly Groundwater Elevation (April 1997 – March 1998).

3.6 Testing and Evaluation Plan

3.6.1 Demonstration Set-Up and Start-Up

There will not be a requirement for mobilization, equipment installation or shakedown for this project. The optimization modelers will visit the sites to collect necessary data, then optimization modeling will be performed by the modelers in their own computer laboratories.

3.6.2 Period of Operation

Optimization modeling will commence at the first demonstration site in February 2001 and will be completed in May 2001. Optimization modeling will be completed at the final site by September 2001. Table 4 shows the proposed schedule through project completion.

Table 4. Project Schedule

Milestone/Deliverable	Completion Date
Select 11 DoD Pump and Treat sites	5/15/00
Apply Pre-optimization screening tool	7/15/00
Select first site for optimization modeling	11/15/00
Summary report of pre-optimization screening results	1/15/01
Complete transport optimization modeling	9/15/01
Summary report of optimization simulation results	7/15/02
Implementation of recommended modifications	4/15/03
Cost and performance report	10/15/03
Tech Transfer package	2/28/03

3.6.3 Amount/Treatment Rate of Material to be Treated

Not applicable to this demonstration.

3.6.4 Residuals Handling

Not applicable to this demonstration.

3.6.5 Operating Parameters for Optimization Modeling

No technology will be operated during this demonstration. Since the demonstration is for PC-based optimization codes, the only operations will be related to computer operations.

However, the optimization modelers will work with a set of constraints and variables to determine the optimal solution to the objective function. At each site, the optimization modeler will be required to solve as many as three mathematical formulations to be defined based on site specific details and requirements. A mathematical formulation consists of a specific objective function coupled with a specific set of constraints. For example, the objective function may be to minimize the total pumping rate from all wells, and constraints might consist of limits on heads, drawdowns, gradients, and pumping rates at individual wells. The project team will develop mathematical formulations based on site-specific data and goals, and subsequently vary these parameters to develop optimal solutions for each formulation.

3.6.6 Experimental Design

The objective of the project is to evaluate the benefits of transport optimization algorithms as a whole, not to evaluate any specific algorithm. Two contracted modelers will independently select and employ transport optimization algorithms (simulated annealing, genetic algorithms, etc.) to solve as many as three mathematical formulations at each of three demonstration sites. The modelers will select algorithms that are the subjects of current research. Many of the codes developed for transport optimization contain multiple algorithms, and the scientists applying the code will determine the most appropriate problem-specific algorithm. The application of these codes will be described in reports or peer-reviewed journals.

The effective experimental approach is maintained by having two independent transport optimization modelers for each site, with a third a third modeler (a contractor from HSI Geotrans) serving as an experimental control by employing traditional, manually iterative optimization techniques, which may include hydraulic modeling, to solve the same set of problems. This approach will result in a robust experimental design.

The demonstration will use existing groundwater flow and transport models for each site. A pre-requisite of selecting a site for the transport optimization simulations is that they have an existing transport model that they consider to be "up-to-date and acceptable for design purposes", based on previous conceptual model development and model calibration activities (which are specifically not within the scope of this project because this project is intended to evaluate the optimization algorithms and not the quality of the underlying transport models). By using existing and valid models, this investigation can focus on the project objective, which is to evaluate the effectiveness of the optimization algorithms given the current modeling resources used by pump and treat installations. Therefore, the costs incurred by the studies will represent only the costs of the optimization analyses without the costs of model development.

The mathematical formulations to be solved at each site will be determined by the ESTCP technical team and also to some extent by constraints imposed by regulations, funding, or logistics at each site. These formulations will include the input of the installations to determine feasibility and usefulness.

Validation of the technology will include a comparison of the current estimated life cycle costs and/or remediation timeframe of the system (collected during the site selection and pre-

optimization screening process) to the life cycle costs and/or remediation timeframe suggested by optimization strategies. It will also include an assessment of the costs associated with actually performing the optimization.

3.6.7 Sampling Plan

Not applicable to this demonstration. No sampling will be performed for this demonstration.

3.6.8 Demobilization

Not applicable to this demonstration.

3.6.9 Health and Safety Plan

Not applicable to this demonstration.

3.7 Selection of Analytical/Testing Methods

Not applicable to this demonstration.

3.8 Selection of Analytical/Testing Laboratory

Not Applicable to this demonstration.

3.9 Management and Staffing

The team members for this project are:

NFESC, Doug Zillmer (PI)	DOE-LLNL, Leah Rogers
NFESC, Paul Lefebvre (Co-PI)	AFBCA, Mario Ierardi
EPA-TIO, Kathy Yager (Co-PI)	AEC, Ira May
USACE, Dave Becker (Co-PI)	Modeling Contractors:
HSI Geotrans, Rob Greenwald	-Richard Peralta, Utah State University
USACE-WES, Jeff Holland	-Chunmiao Zheng, University of Alabama

The management structure is illustrated in Figure 11, below.

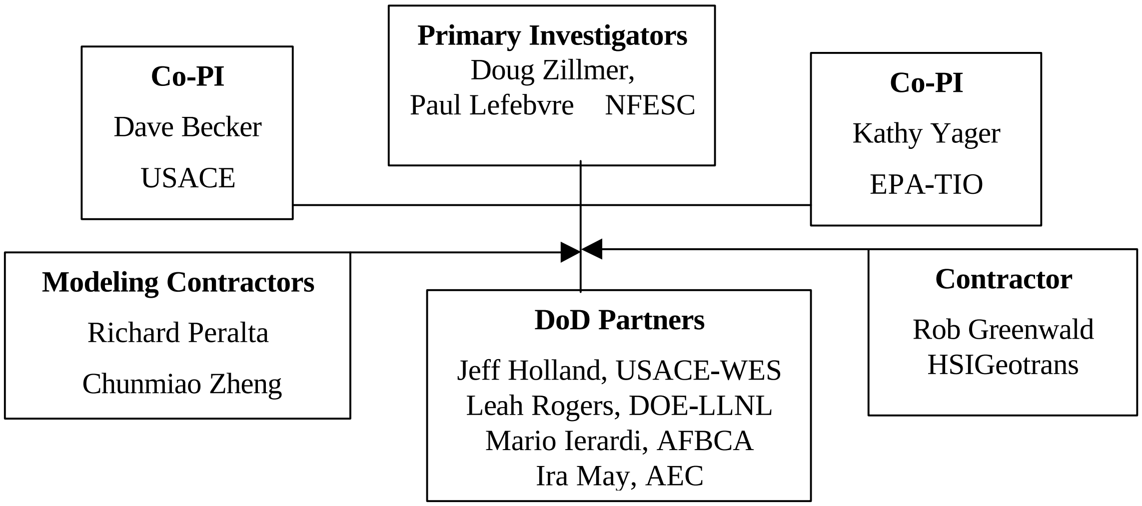

Figure 11. Management Structure Wiring Diagram

3.10 Demonstration Schedule

See Section 3.6.2 (including Table 4).

4. Performance Assessment

4.1 Performance Criteria

Primary and secondary performance criteria for the optimization analyses are presented in Table 5. These criteria will be applied to the results from each of the optimization analyses, those using algorithms and those done manually. As described in Section 4.2, the primary criteria are quantitative, while the secondary criteria are qualitative.

Table 5. Performance Criteria

Performance Criteria	Description	Primary or Secondary
Reduce annual operating costs	Does demonstration indicate potential for reducing annual operating costs (based on modeling)?	Primary
Faster remediation	Does demonstration indicate potential for increased contaminant removal (based on modeling)?	Primary
Reduce life cycle cost of system	Does demonstration indicate potential for reduced life cycle based on capital costs, modified annual costs, and modified operating (based on modeling)?	Primary
Factors Affecting Technology Performance	Extent to which site-specific factors affect technology performance (or prohibit application of the technology), such as reliability of models, confidence in plume delineation, confidence in source area delineation, etc.	Secondary
Ease of Use	What is the required skill level and training required to apply the technology at other sites, and can others be expected to apply technology as effectively (and for similar cost) as the project team for this demonstration project?	Secondary

4.2 Performance Confirmation Methods

The objective of this project is to demonstrate the cost benefit of applying transport optimization codes for three existing pump and treat systems. For each site, up to three mathematical formulations will be constructed and solved. Each mathematical formulation consists of an equation to be maximized or minimized, and a set of constraints that must all be satisfied.

Examples of objective functions are:

- minimize total cost over 20 years
- minimize cleanup time
- maximize the mass of contaminant removed

Examples of constraints are:

- TCE is less than 5 ppb after 20 years
- Total pumping rate < 500 gpm
- drawdown at a specific location is < 2 ft

The mathematical nature of this project is ideal for evaluating the performance of the transport optimization technology. This is because the optimization is based on achieving the "best" value of the objective function, which is a mathematical equation for which a value can be calculated. This allows a quantitative assessment of performance.

Primary performance criteria will be assessed based on values of the objective function for competing solutions (where each solution is a specific combination of pumping locations and pumping rates). Objective function values can be calculated for the present system, a revised system suggested by transport optimization codes/algorithms, and a revised system determined with modeling but without transport optimization codes/algorithms (see section 4.3). The secondary performance criteria, and associated metrics, are qualitative rather than quantitative. Table 6 shows the primary and secondary performance criteria along with expected performance metrics and performance confirmation methods. Because post-modeling adjustments are beyond the scope of this study, performance evaluation will rely on modeling results only and not data from future adjustments (though any future modifications will be tracked and subsequently reported).

Table 6. Expected Performance and Performance Confirmation Methods

Performance Criteria	Expected Performance Metric (pre-demo)	Performance Confirmation Method
Primary Criteria (Quantitative)		
Reduce annual operating costs	> 20%	Objective function and/or constraint set
Faster remediation	> 20%	Objective function and/or constraint set
Reduce life cycle cost of system	> 20%	Objective function and/or constraint set
Secondary Criteria (Qualitative)		
Factors Affecting Performance	No pre-demo metrics assumed	Experience from three demonstration sites
Ease of Use	Useful to professionals who are capable of executing	Experience from three demonstration sites

	transport simulation models	

4.3 Data Analysis, Interpretation, and Evaluation

As previously stated, the mathematical nature of this project is ideal for evaluating the performance of the transport optimization technology. This is because the optimization is based on achieving the “best” value of the objective function, which is a mathematical equation for which a value can be calculated. Therefore, a pre-optimization value of the objective function can be calculated for each optimization formulation (based on the current system), and alternative solutions determined using the transport optimization techniques can be evaluated with respect to the pre-optimization solution by comparing the respective objective function values.

Two independent groups will solve each mathematical formulation, using different transport optimization codes/algorithms. Each group will be given the same amount of time, and be provided with the same underlying transport model. The optimal objective function values computed by each group will be compared to evaluate the relative strengths of each code/algorithm. Furthermore, an additional control analysis will be performed to allow the true benefits of the optimization techniques to be evaluated. The control study will utilize a traditional, manually iterative optimization, to be performed independently and within the same schedule. The traditional optimization will be performed by HSI Geotrans, and may incorporate the use of hydraulic optimization tools (e.g., MODMAN Version 4.0) to solve surrogate optimization problems that are based only on groundwater flow components. However, the control study will be based on the same transport model, objective functions, and constraint sets solved by the two groups of transport optimization modelers. The only difference between the control study group and the two transport optimization groups will be the use of the optimization codes/algorithms by the transport optimization groups. Therefore, the net benefit provided by those codes/algorithms can be evaluated, as measured by the optimal objective function values achieved by each independent group.

As previously stated, all results from this project will be based on existing transport simulation models. It will be up to the individual installations to determine if the results merit actual field implementation. As with any design based on a simulation model, actual field results may differ from model calculated results once a specific solution is implemented in the field. Although that is clearly not within the control of the project team, the issue is dealt with (to the extent possible) by only selecting demonstration sites where the transport simulation is described as “currently used for design purposes”.

5. Cost Assessment

5.1 Cost Reporting

This project will demonstrate the cost benefit of applying computer-based transport optimization codes, and therefore, the cost reporting will differ from other ESTCP cleanup technology demonstration projects. Some typical cost tracking categories (Start-Up Costs, Capital Costs, Indirect Environmental Activity Costs, and Demobilization) will not apply. The majority of the costs related to this demonstration will be labor costs of the modelers. There are no capital costs associated with this demonstration since the optimization codes and existing models will run on standard PCs.

Two transport optimization modelers (contractors) have been selected to perform optimization analyses on each of the three technology demonstration sites (i.e., a total of six applications of the technology). For each site, the optimization modelers will track the level of effort, and the corresponding costs, associated with each of the following tasks:

- Pre-Optimization Tasks
- Optimization Modeling
- Reporting

After the demonstration has been completed at all three sites, each modeler will report costs for each task and at each site. In addition, the modelers will be asked to explain whether the costs represent the anticipated range of expected costs for other sites where the technology might be applied. This will meet the ESTCP goal of developing and validating the expected operational cost of the demonstrated technology.

5.2 Cost Analysis

5.2.1 Cost Comparison

The cost benefit of applying transport optimization codes will be determined by comparing costs of the following:

- applying the innovative technology (transport optimization techniques)
- applying the baseline alternative technology (traditional optimization using manually iterative techniques), and
- the cost of operating the system in its current state.

The life cycle cost savings of optimization will be estimated by adding the costs of applying the optimization techniques to the sum of the incremental life cycle cost of any changes to the systems configuration (e.g. add additional extraction well, decrease total pumping rate by 10%, reduce duration of remediation).

5.2.2 Cost Basis

The basis for estimating costs for future applications of the technology is anticipated to be one to two hours for each transport simulation to execute, and 1 or 2 constituents that must be simulated to provide adequate information for management decisions. These are significant cost drivers for this technology. The adequacy of assumptions stated above regarding simulation time and chemical constituents will be assessed during the technology demonstrations at the three sites. The final report will discuss the extent to which these assumptions are likely to apply at others sites.

5.2.3 Cost Drivers

The anticipated cost drivers for the transport optimization modeling is the model execution time for simulating a chemical constituent, and the number of chemical constituents that must be simulated to adequately address the plume management issues at the site.

5.2.4 Life Cycle Costs

The transport optimization technology is generally applied over a short duration (less than two years). Therefore, life-cycle costs of the technology are essentially equivalent to the costs of applying the technology (see Section 5.1 for a discussion of how the costs of applying the technology will be tracked).

6. Implementation Issues

6.1 Environmental Checklist

The work required for this demonstration, which involves computer simulations, is not subject to specific regulations and does not require any permits.

6.2 Other Regulatory Issues

At each of the three demonstration sites, potential modifications to an existing pump and treat system will be suggested by the results. These may include changes in pumping rates at existing wells, or additional locations for pumping and/or injection. The specific installations will determine whether or not results from the demonstration project merit actual changes to the existing system, which would require subsequent regulatory interaction. At the request of the installation, one or more members of the project team will present the site-specific findings of the demonstration project to regulators after final results are obtained.

6.3 End User Issues

The end-users for transport optimization codes will be experienced transport modelers. It is anticipated that cleanup site managers will utilize modelers to implement optimization codes for the optimization of pump and treat systems. Commercial-off-the-shelf computer systems can be used to implement optimization codes. The optimization codes demonstrated during this project will be accessible, free of charge to authorized users, through the DoD Groundwater Modeling System (GMS). It will not be necessary to customize the optimization codes for this demonstration or for future end-user requirements, but objective functions will be customized for each site to meet site-specific requirements.

7. References

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Appendix C: Outline for Training Courses

Draft Outline
Technical Training, Computer Modeling Optimization

- ***first day of class for all; managers and technical staff***

1. Introductions and Overview
   a. Students
   b. Instructors
   c. Overview of course
   d. Objectives
      - Describe benefits of computer modeling optimization
      - Identify sites which can benefit from application of such numerical optimization
      - Describe the process of numerical optimization
      - Identify needed information for optimization
      - Generally describe technical basis for the optimization algorithms and means to select between them
      - Introduce two existing packages for optimization

2. Why Perform Optimization of Ground Water Extraction Systems
   a. Overview of aspects of optimization of ground water extraction systems
   b. Purpose of computer modeling optimization and definition of optimization
   c. Previous demonstrations of computer modeling optimization
   d. Potential cost savings
   e. What sites can benefit from application of such optimization?
   f. What is needed for computer modeling optimization?
   g. Who can do computer modeling optimization, what support is needed?

3. Numerical Optimization Process
   a. Determine optimization objectives
   b. Verify underlying ground water flow/transport model adequacy
   c. Select optimization package
   d. Develop formulations
      - define "formulation," "objective function," and ”constraint"
      - develop objective functions
      - identify constraints
   e. Program formulation
   f. Conduct optimization (expertise required)
   g. Interact with project team with initial results to focus optimization
   h. Consolidate and report results
   i. Revisit optimization periodically during operations

4. Developing Formulations
   a. Clarifying objectives
   b. Develop objective functions that meet project decision needs
      - minimize cost over time (with or without discounting)

- minimize time to reach goal
- minimize flow rate (subject to constraints)
- maximize mass removal/minimize mass remaining
- must identify cost dependencies and functions for all significant costs

c. Identify constraints
- cost constraints
- time constraints
- concentration constraints
- containment constraints
- flow constraints
- location constraints

d. Project team involvement

e. Optimizers' role in formulation development

5. Numeric Optimization Algorithms
   a. Purpose - generally describe how algorithms work
   b. Genetic algorithm
   c. Simulated annealing
   d. Taboo search
   e. Other enhancements
      - response function development
      - artificial neural networks

6. Optimization Packages
   a. SOMOS1 and SOMOS3
   b. MGO
   c. Others
   d. Differences

7. First Day Wrap Up

- ***Second day of class - primarily for technical staff and modelers***

8. Approach to Optimization
   a. Reducing run times by limiting universe of options for locations and pumping rates
   b. Which problem to try first? Learning from initial runs.
   c. Breaking the problem into pieces
   d. When to use response functions instead of "brute force"

9. Hands-On Use of Optimization Tools

   a. Sample formulation problem
   b. Develop Input
   c. Look at output
   d. Hands-on demonstration of simple problems

10. Second Day Wrap Up

The following Appendices are in Volumes II and III:

Within Volume II:
Appendix D: Formulation Document and Final Reports, Umatilla
Appendix E: Formulation Document and Final Reports, Tooele
Appendix F: Formulation Document and Final Reports, Blaine

Within Volume III:
Appendix G: Phase 1 Demonstration Plan and Pre-Optimization Screening Draft Report